

# Topological insulators and K-theory

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## Abstract

We analyze the topological  $\mathbb{Z}_2$  invariant, which characterizes time reversal invariant topological insulators, in the framework of index theory and K-theory. The topological  $\mathbb{Z}_2$  invariant counts the parity of Majorana zero modes, which can be interpreted as an analytical index. So it fits perfectly into an index theorem, and the topological index provides an efficient way to compute the topological  $\mathbb{Z}_2$  invariant. Finally, the bulk-boundary correspondence gives a different perspective to view the index theorem of the topological  $\mathbb{Z}_2$  invariant.

## 1 Introduction

A time reversal invariant topological insulator, or simply topological insulator [17], of free or weak-interacting fermions is a system that has both time reversal  $\mathbb{Z}_2$  symmetry and charge conservation (a  $U(1)$  symmetry). Accordingly, in the framework of symmetry protected topological (SPT) phases [10], topological insulators are also referred to as  $U(1)$  and time reversal symmetry protected topological order. In this work, we are mainly interested in time reversal invariant fermionic systems in a crystal. According to the Altland-Zirnbauer-Cartan classification of general topological insulators with different

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symmetries [1, 29], topological insulators with time reversal symmetry are in the symplectic class, which is referred to as type AII topological insulators.

Time reversal invariant topological insulators can be characterized by a  $\mathbb{Z}_2$ -valued topological invariant originally derived from quantum field theory [19, 26], which basically counts the parity of Majorana zero modes. Majorana zero modes [28] are quasiparticle excitations bound to a defect at zero energy. Two Majorana zero modes can couple together and behave as an effective composite boson. For example, Dirac cones are Majorana zero modes in three dimensional (3d) time reversal invariant systems, and the presence of an unpaired Dirac cone is the characteristic of a 3d non-trivial topological insulator. We have to point out that Majorana zero modes should not be confused with Majorana spinors. Majorana spinors have been understood by the representation theory of Clifford algebras and the geometry of spinors (i.e., spin geometry) [25]. In contrast, the concept of Majorana zero modes is new in mathematical physics, and they have a different representation theory and geometry compared to Majorana spinors.

Physicists originally proposed two ways to define a  $\mathbb{Z}_2$ -valued topological invariants using different perspectives. The Kane–Mele invariant was first defined in the quantum spin Hall effect in graphene [19], and subsequently generalized to 3d topological insulators [14]. It is defined as the product of the signs of Pfaffians over the fixed points of the time reversal symmetry. In contrast to the discrete Pfaffian formalism of the Kane–Mele invariant, the Chern–Simons invariant has an integral form defined by the variation of Chern–Simons actions under a specific gauge transformation induced by the time reversal symmetry [26]. In string theory, the Chern–Simons invariant is also called the Wess–Zumino–Witten (WZW) topological term. The WZW term is an action functional in gauge theory, and the Kane–Mele invariant is derived from an effective fermionic field theory. In fact, the Kane–Mele invariant and the Chern–Simons invariant are equivalent, so we view them as different aspects of the same  $\mathbb{Z}_2$  invariant, and we call both of them the topological  $\mathbb{Z}_2$  invariant.

In this work, we will explain that the topological  $\mathbb{Z}_2$  invariant can be simply understood via a mod 2 index theorem derived from a time reversal invariant Hamiltonian. More precisely, first, the analytical  $\mathbb{Z}_2$  index of the effective Hamiltonian can be interpreted as the mod 2 spectral flow of chiral zero modes, which counts the parity of Majorana zero modes. And secondly, the analytical  $\mathbb{Z}_2$  index via the index theorem can be computed by a topological  $\mathbb{Z}_2$  index based on the Chern character.

In order to understand the mod 2 index theorem, we look into the  $K$ -theory and  $K$ -homology of topological insulators, since this is the right framework to study index theory. If one considers the band structure of a fermionic system in a crystal, one is actually working on the Hilbert bundle over its momentum space, which is also called the Brillouin zone in condensed matter physics. Taking time reversal symmetry into account, the Hilbert bundle becomes a Quaternionic vector bundle equipped with (anti-)involutions. So the Quaternionic  $K$ -theory, i.e.,  $KQ$ -theory, can be used to classify all possible band structures of a topological insulator of type AII. Furthermore, the topological  $\mathbb{Z}_2$  invariant is a mod 2 index obtained from the pairing between  $KQ$ -theory and  $KQ$ -homology.

As an instance of the holographic principle, the bulk-boundary correspondence gives rise to an isomorphism between the bulk  $K$ -theory and the boundary  $K$ -theory. For a topological insulator, the bulk is the momentum space, and the role of the boundary is played by the fixed points of the time reversal symmetry. As we argue, the bulk-boundary correspondence of a topological insulator realizes the same mod 2 index theorem from a different point of view.

In this work, we give a complete explanation of the topological  $\mathbb{Z}_2$  invariant in the framework of index theory and  $K$ -theory. We provide the following list of new results on topological insulators:

- By comparing the geometry of Majorana zero modes with  $KR$ -cycles of Majorana spinors, we model Majorana zero modes by generalized  $KR$ -cycles or  $KQ$ -cycles in analytical  $KR$ -homology. (Recall that  $KQ$  and  $KR$  are related by  $KQ^{-j}(X) = KR^{-j-4}(X)$ .)
- By extending a time reversal invariant Hamiltonian to the effective Hamiltonian acting on Majorana states, we interpret the topological  $\mathbb{Z}_2$  invariant as a mod 2 analytical index.
- We give an explanation of the topological  $\mathbb{Z}_2$  invariant based on the  $K$ -theoretic interpretation of the topological index.
- We derive the equivalence between the Chern–Simons invariant and the Kane–Mele invariant for 3d topological insulators.
- We explore the bulk-boundary correspondence of a topological insulator at the level of  $K$ -theory.

This article is organized in the following way. As an introduction to KQ-theory, we review some relevant facts and give some basic examples in section 2. Section 3 focuses on the analytical theory of Majorana zero modes, and the topological  $\mathbb{Z}_2$  invariant is interpreted as a mod 2 analytical index. In section 4, the mod 2 analytical index is computed by a mod 2 topological index. Finally, the bulk-boundary correspondence of a topological insulator is briefly discussed in 5.

## 2 KQ-theory

In this section, we will first introduce the  $\mathbb{Z}_2$  time reversal symmetry and model the band structure of a time reversal invariant topological insulator by its Hilbert bundle, which is a Quaternionic vector bundle over a Real space. In order to classify all possible band structures of a topological insulator, we will apply the Quaternionic K-theory, i.e.,  $KQ$ -theory, which is equivalent to the Real K-theory, i.e.,  $KR$ -theory. Finally, the real Baum–Connes isomorphism for the free discrete group  $\mathbb{Z}^d$  will be briefly reviewed as a preparation for further discussions in the last section.

### 2.1 Time reversal symmetry

Let  $X$  be a compact space, which will be viewed as the momentum space of the lattice model of a topological insulator.

**Example 1.** A lattice in  $\mathbb{R}^d$  is a free abelian group isomorphic to  $\mathbb{Z}^d$  and its Pontryagin dual is the torus  $\mathbb{T}^d$ , the simplest and most important example of a momentum space is  $X = \mathbb{T}^d$ .

**Example 2.** The limit of a lattice model is the continuous model defined on  $\mathbb{R}^d$  and its Pontryagin dual is itself, in this case the momentum space is the one point compactification of  $\mathbb{R}^d$ , i.e.,  $X = (\mathbb{R}^d)^+ = \mathbb{S}^d$ .

**Definition 1.** An involutive space  $(X, \tau)$  is a compact space  $X$  equipped with an involution, i.e., a homeomorphism  $\tau : X \rightarrow X$  such that  $\tau^2 = id_X$ .

As a convention,  $(X, \tau)$  is also called a Real space since the involution  $\tau$  is usually taken as the complex conjugation, which was first introduced by Atiyah in the Real K-theory, i.e.,  $KR$ -theory [2].

Time reversal symmetry is a fundamental symmetry of physical laws, which is the  $\mathbb{Z}_2$  (as a notation  $\mathbb{Z}_2 \cong \mathbb{Z}/2\mathbb{Z}$ ) symmetry defined by the time reversal transformation  $\tau : t \mapsto -t$  reversing the direction of time. The effect of the time reversal transformation on a momentum space is to change the sign of its coordinates basically because  $\tau$  changes the sign of the imaginary unit  $\tau : i \mapsto -i$ .

**Definition 2.** Time reversal symmetry defines the time reversal transformation on the momentum space  $X$ ,

$$\tau : X \rightarrow X; \quad x \mapsto \tau(x)$$

so that  $(X, \tau)$  is an involutive space.

The time reversal transformation may vary according to the choice of coordinate system on  $X$ .

**Example 3.** The unit sphere  $\mathbb{S}^d$  in Cartesian coordinates is

$$\mathbb{S}^d = \{(x_0, x_1, \dots, x_d) \in \mathbb{R}^{d+1} \mid x_0^2 + x_1^2 + \dots + x_d^2 = 1\}$$

the time reversal transformation on  $\mathbb{S}^d$  is defined by

$$\tau : \mathbb{S}^d \rightarrow \mathbb{S}^d; \quad (x_0, x_1, \dots, x_d) \mapsto (x_0, -x_1, \dots, -x_d)$$

so the unit sphere under this involution is also denoted by  $\mathbb{S}^{1,d} \subset \mathbb{R}^{1,d}$ .

**Example 4.** If the torus  $\mathbb{T}^d$  is parametrized by the angles

$$\mathbb{T}^d = \{(e^{i\theta_1}, \dots, e^{i\theta_d}) \mid \theta_i \in [-\pi, \pi] \bmod 2\pi, i = 1, \dots, d\}$$

then the time reversal transformation on  $\mathbb{T}^d$  is defined by

$$\tau : \mathbb{T}^d \rightarrow \mathbb{T}^d; \quad (e^{i\theta_1}, \dots, e^{i\theta_d}) \mapsto (e^{-i\theta_1}, \dots, e^{-i\theta_d})$$

The fixed points of an involution  $\tau$  is the set of points

$$X^\tau := \{x \in X \mid \tau(x) = x\}$$

**Example 5.** The unit sphere  $\mathbb{S}^d$  has 2 fixed points under the time reversal transformation,  $(\mathbb{S}^d)^\tau = \{(\pm 1, 0, \dots, 0)\}$ .

**Example 6.** The torus  $\mathbb{T}^d$  has  $2^d$  fixed points under the time reversal transformation,  $(\mathbb{T}^d)^\tau = \{(\pm 1, \pm 1, \dots, \pm 1)\}$  when  $\theta_i = 0, \pi$ .

The involutive space  $(X, \tau)$  has the structure of a  $\mathbb{Z}_2$ -CW complex, that is, there exists a  $\mathbb{Z}_2$ -equivariant cellular decomposition of  $X$ , which will be discussed in detail later on. In the other way around, starting with the fixed points  $X^\tau$ ,  $X$  can be built up by gluing cells that carry a free  $\mathbb{Z}_2$  action, i.e.,  $\mathbb{Z}_2$ -cells. Such equivariant cellular decomposition is very useful in the computation of K-theory. This construction is closely related to the stable splitting of  $X$  into spheres respecting the time reversal symmetry [13].

**Definition 3.** A Quaternionic vector bundle  $(E, \chi)$  over an involutive space  $(X, \tau)$  is a complex vector bundle  $E$  over  $X$  with an anti-linear anti-involution  $\chi$  (that is compatible with  $\tau$ ). The anti-involution  $\chi$  is an anti-linear bundle isomorphism  $\chi : E \rightarrow E$  such that  $\chi^2 = -id_E$ .

In the above definition, if the anti-involution  $\chi$  (s.t.  $\chi^2 = -1$ ) is replaced by an involution  $\iota$  (s.t.  $\iota^2 = 1$ ), then  $(E, \iota)$  is a Real space and the pair  $(E, \iota)$  defines a Real vector bundle over  $(X, \tau)$ .

For a Quaternionic vector bundle  $\pi : (E, \chi) \rightarrow (X, \tau)$ , the compatibility condition between  $\chi$  and  $\tau$  is obviously  $\pi \circ \chi = \tau \circ \pi$ . For any section  $s : (X, \tau) \rightarrow (E, \chi)$ , the above compatibility condition implies that for any  $x \in X$ ,  $s \circ \tau(x)$  and  $\chi \circ s(x)$  are in the same fiber. In order to compare two sections, we define an action  $\varsigma$  on the space of sections  $\Gamma(X, E)$ ,

$$\varsigma : \Gamma(X, E) \rightarrow \Gamma(X, E); \quad s \mapsto -\chi \circ s \circ \tau$$

$\varsigma$  is itself an anti-involution such that  $\varsigma^2 = -1$ . The negative sign in the definition of  $\varsigma$  comes from the anti-involution  $\chi$  in the following way. Comparing the above two sections, one would have the difference  $s \circ \tau - \chi \circ s$ . Moving this back to the original fiber by applying  $\chi$ , the difference becomes  $\chi \circ s \circ \tau + s = s - \varsigma(s)$ .

At a fixed point  $x \in X^\tau$ , the restriction  $\chi_x : E_x \rightarrow E_x$  is an anti-linear map such that  $\chi_x^2 = -1$  so that  $\chi_x$  gives a quaternionic structure on  $E_x$ , i.e. a fiber preserving action of the quaternions. If the complex dimension of  $E_x$  is even, say  $\dim_{\mathbb{C}} E_x = 2n$ , then  $E_x$  can be viewed as a vector space defined over the quaternions  $\mathbb{H}$  with quaternionic dimension  $\dim_{\mathbb{H}} E_x = n$ . From now on, we assume that the Quaternionic vector bundle  $(E, \chi)$  has even rank, say  $\text{rank}(E) = 2n$ . Let  $i : X^\tau \hookrightarrow X$  be the inclusion map, when restricting  $E$  to

the set of fixed points,  $i^*E \rightarrow X^\tau$  turns into a quaternionic vector bundle, i.e., each fiber is a quaternionic vector space. The reader should not confuse quaternionic vector bundles with Quaternionic vector bundles.

**Definition 4.** A complex vector bundle is said to be a Hilbert bundle if each fiber is a Hilbert space, i.e., a complex vector space equipped with a complete Hermitian inner product. The completeness is automatic in the finite dimensional case.

A Hilbert bundle (with a flat connection) was introduced to model fields of Hilbert spaces in geometric quantization, for example see [6]. Given a time reversal invariant Hamiltonian  $H$  of a topological insulator, let us consider the corresponding Hilbert bundle  $\pi : \mathcal{H} \rightarrow X$ , which describes the band structure of the topological insulator over the momentum space  $X$ . The space of states (in the momentum representation) is then given by the Hilbert space of (local) sections  $\mathcal{H} = \Gamma(X, \mathcal{H})$  with fiber-wise inner product.

Over the fixed points  $X^\tau$ , if an inner product is chosen on the quaternionic vector bundle  $i^*E \rightarrow X^\tau$ , i.e., a Hilbert bundle with the quaternionic structure induced by  $\chi$ , then it naturally gives rise to a symplectic structure  $\omega$  so that  $(i^*E, \omega) \rightarrow X^\tau$  becomes a symplectic vector bundle, i.e., each fiber is a symplectic vector space, see e.g. [23][3.3.1].

### 2.1.1 Hilbert space description

Time reversal symmetry can be represented by the time reversal operator  $\Theta$  acting on the Hilbert space  $\mathcal{H}$ . And the time reversal operator is a product  $\Theta := UC$ , where  $U$  is a unitary operator and  $C$  is the complex conjugation [31]. Hence,  $\Theta$  is an anti-unitary operator, that is, for  $\psi, \phi \in \Gamma(X, \mathcal{H})$ ,

$$\langle \Theta\psi, \Theta\phi \rangle = \overline{\langle \psi, \phi \rangle} = \langle \phi, \psi \rangle, \quad \Theta(a\psi + b\phi) = \bar{a}\Theta\psi + \bar{b}\Theta\phi, \quad a, b \in \mathbb{C}$$

Since  $\Theta$  is acting on fermionic states, it has the important property  $\Theta^2 = -1$ , so  $\Theta$  is a skew-adjoint operator, i.e.,  $\Theta^* = -\Theta$ . These properties also imply that  $\langle \phi, \Theta\phi \rangle = 0$ .

The action of time reversal symmetry on the momentum space  $X$  (i.e., in momentum representation) is given by  $x \mapsto \tau(x)$ . The time reversal symmetry lifts to an anti-linear anti-involution  $\chi_\Theta$  on the Hilbert bundle  $\mathcal{H} \rightarrow X$  via the identity  $\chi_\Theta(\phi(x)) = (\Theta\phi)(x) = \phi(\tau(x))$  and vice-versa. In the following, by abuse of notation, we will denote  $\chi_\Theta$  simply by  $\Theta$ .

A time reversal invariant Hamiltonian family  $H = H(x)$  must satisfy the condition

$$\Theta H(x) \Theta^* = H(\tau(x)) \quad \text{for any } x \in X \quad (1)$$

For an eigenstate  $\phi$  with  $H(x)\phi(x) = E_\phi(x)\phi(x)$ , we have

$$\Theta H(x) \Theta^* \Theta \phi(x) = H(\tau(x)) \phi(\tau(x)) = E_\phi(\tau(x)) \phi(\tau(x)) = E_\phi(\tau(x)) \Theta \phi(x)$$

On the other hand,

$$\Theta[H(x)\phi(x)] = \Theta[E_\phi(x)\phi(x)] = \Theta E_\phi(x) \Theta \phi(x) = E_{\Theta\phi}(x) \Theta \phi(x)$$

Hence the eigenvalue of  $\Theta\phi$  satisfies  $E_{\Theta\phi}(x) = \Theta E_\phi(x) = E_\phi(\tau(x))$ . This means that the linearly independent eigenstates  $\phi$  and  $\Theta\phi$  take on the same eigenvalue  $E$  at  $x$  respectively  $\tau(x)$ . This is what is called Kramers' degeneracy. The pair  $(\phi, \Theta\phi)$  is called a Kramers pair.

Taking time reversal symmetry into account, the Hilbert bundle over the momentum space  $\pi : \mathcal{H} \rightarrow X$  becomes a Quaternionic Hilbert bundle  $\pi : (\mathcal{H}, \Theta) \rightarrow (X, \tau)$ , where  $\tau$  is the time reversal transformation on the base space such that  $\tau^2 = id_X$  and  $\Theta$  is the time reversal operator which satisfies  $\Theta^2 = -id_{\mathcal{H}}$ .

### 2.1.2 Induced structures and Kramers pairs

The following facts are discussed in detail in [23]. With time reversal symmetry the rank of the Hilbert bundle  $\mathcal{H}$  can be always assumed to be even, say  $rank(\mathcal{H}) = 2N$ . We always assume that the fiberwise action of  $\Theta$  on the Hilbert bundle is non-degenerate outside the fixed points, and that the only degeneration at the fixed points is due to Kramers' degeneracy, that is, due to  $\Theta$  acting fiberwise over  $X^\tau$ . Then, there exists a decomposition

$$\mathcal{H} = \bigoplus_{i=1}^N \mathcal{H}_i \quad (2)$$

where  $\mathcal{H}_i \rightarrow X$  is a rank 2 subbundle, see e.g. [23]. We set  $\mathcal{H}_i = \Gamma(X, \mathcal{H}_i)$ , then  $\mathcal{H} = \bigoplus_{i=1}^N \mathcal{H}_i$  and  $\Theta$  respects this decomposition.

Outside of the fixed points  $X^\tau$ , we can locally trivialize the bundle using Kramers pairs. By assumption that the Kramers' degeneracies are the only degeneracies, it follows that on  $X \setminus X^\tau$  the bundle  $\mathcal{H}_i$  splits into a direct sum of two line bundles:  $\mathcal{H}_i|_{X \setminus X^\tau} = \mathcal{L}_{2i-1} \oplus \mathcal{L}_{2i}$ . Thus if we choose trivializing



sections  $\psi_{2i-1}, \psi_{2i}$  on some neighborhood  $U$  with  $U \cap \tau(U) = \emptyset$ , then we obtain a Kramers pair  $(\psi_I, \psi_{II})$ ,  $\psi_{II} = \Theta\psi_I$  given by

$$\psi_I|_U = \psi_{2i-1}, \quad \psi_I|_{\tau(U)} = \Theta\psi_{2i} \text{ and } \psi_{II}|_U = -\psi_{2i}, \quad \psi_{II}|_{\tau(U)} = \Theta\psi_{2i-1} \quad (3)$$

On  $X^\tau$  by definition Kramers pairs are linearly independent and trivialize the bundle  $\mathcal{H}_i|_{X^\tau}$ .

Thus we see that Kramers pairs span outside of  $X^\tau$  and on  $X^\tau$ . The interesting part is the interplay between the two, which is the origin of the  $\mathbb{Z}_2$  invariant. To further analyze this, we will now decompose the underlying space  $X$  according to the action by  $\tau$ . We will assume that the Real space  $(X, \tau)$  is *tame*. For a connected  $X$  this means that there are closed connected fundamental domains  $V_\pm$ , such that  $\tau(V_\pm) = V_\mp$ ,  $X = V_+ \cup V_-$  and  $B = V_+ \cap V_-$  is the closed boundary of both  $V_+$  and  $V_-$ . That is  $V_\pm = V_\pm^o \amalg B$  as sets, with  $\tau(V_\pm^o) = V_\mp^o$  open and  $B$  is closed of codimension greater or equal to 1. Such  $B$  separates, namely,  $V_+^o$  and  $V_-^o$  occupy different components of  $X \setminus X^\tau$ . Here and in the following  $\amalg$  means the disjoint union. For general  $X$ , tame means that each connected component of  $X$  is tame. This is for instance the case for a Riemannian manifold  $X$  where  $V_\pm$  are given by Dirichlet fundamental domains, a.k.a., Voronoi cells. We call a tame space *regular*, if we can find a decomposition  $X = X_+ \amalg X_- \amalg X^\tau$  where  $\tau X_\pm = X_\mp$  such that  $\bar{X}_\pm = V_\pm$  and  $X_\pm$  and  $X \setminus X^\tau$  are locally compact. This is the case for all the examples that we will consider including the Examples above. See Figure 1.

Another class, which is the most important for applications is when  $(X, \tau)$  is a finite  $\mathbb{Z}_2$ -equivariant regular CW complex. This means that for all cells  $C$  of dimension  $k$ ,  $\tau(C)$  is also a cell of dimension  $k$ . In this case, we can decompose  $X = V_+ \cup V_-$  as above where now  $V_\pm$  are sub CW complexes. Moreover,  $V_\pm = \bar{O}_\pm$  where  $O_\pm = \amalg_{C \in V_\pm} C^o$  is the union of all the interiors of the top dimensional cells in  $V_\pm$ , that is, those that are not at the boundary of any other cell. We denote the closed cells by  $C$  and write  $C^o$  for their open interior. There is also another decomposition, which we will use  $X = X_+ \amalg X_- \amalg X^\tau$ . To do this, we assign  $+$ ,  $-$  or *fix* to all cells, inductively, by choosing fundamental domains as above starting with the dimension zero cells and using induction on the  $k$ -skeleton. We choose  $+$  and  $-$  for the cells interchanged by  $\tau$  and *fix* for all the cells fixed by  $\tau$ . We will call them  $+$ ,  $-$  or fixed cells. The induction ensures that no  $+$  cell lies at the boundary of only  $-$  cells. Notice that fixed points do not lie in the interior of any  $+$  or  $-$

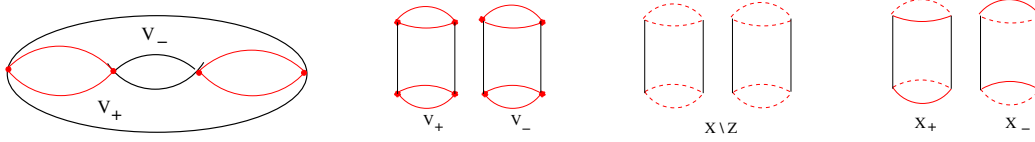


Figure 1: The torus with two fundamental domains  $V_+, V_-$  with  $Z = V_+ \cap V_- = \mathbb{S}^{1,1} \amalg \mathbb{S}^{1,1}$  in red, the disjoint union of  $V_+$  and  $V_-$ , the complement of  $Z$ , and the subsets  $X_\pm$ . Dotted lines indicate open boundaries.

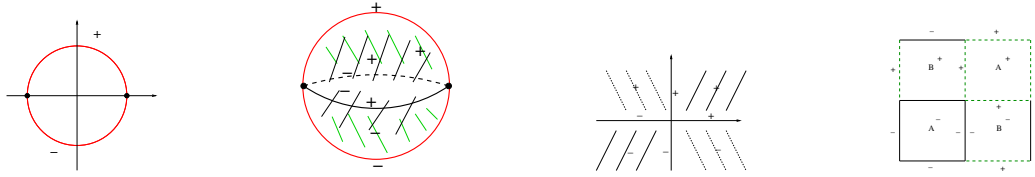


Figure 2: The weak FKMM decompositions of (a)  $\mathbb{S}^{1,1}$ , (b)  $\mathbb{S}^{1,2}$ , with 2 0-cells, 4 1-cells and 4 2-cells, corresponding to the one-point compactification of  $\mathbb{R}^{0,2}$  decomposed into quadrants and half lines depicted in (c), and (d) the decomposition of  $\mathbb{T}^2$ .

cell, moreover,  $X^\tau = \amalg_{C:\text{fixed cell}} C^o$ . Set  $X_+ = \amalg_{C: + \text{ cell}} C^o$ ,  $X_- = \amalg_{C: - \text{ cell}} C^o$ . Building on nomenclature of [12], we call such a CW complex of *weak FKMM type* if there is a choice of  $\pm$  such that each skeleton  $X^k$  is regular, as defined above, with respect to the decomposition above. This is for instance the case, if  $X$  is a compact manifold and  $X^\tau$  is discrete, which encompasses all the examples from the literature. In particular this means that if  $Z = V_+ \cap V_-$  then  $Z$  is again of weak FKMM type and one can use induction.

**Example 7.** All the  $\mathbb{T}^d$  and  $\mathbb{S}^{1,d}$  are of this type. For  $d = 0$  the space consists of two points, marked by *fix*. For  $d = 1$  one adds two intervals joining the points, marked by  $+$  and  $-$ . For  $\mathbb{S}^d$ , we realize it as  $\mathbb{R}^{0,d} \cup \{\infty\}$ . Mark  $\infty$  by *fix* and then mark  $\mathbb{R}^{0,d}$  by decomposing it w.r.t. the iterated upper and lower half spaces, marking the upper half space by  $+$  and the lower by  $-$ . This agrees with the decomposition as  $\mathbb{R}^{0,d} = \mathbb{R}^{0,1} \times \dots \times \mathbb{R}^{0,1}$ . Similarly, we can define the decomposition of  $\mathbb{T}^d = \mathbb{S}^{1,1} \times \dots \times \mathbb{S}^{1,1}$ , see Figure 2.

Under the tameness assumption above we can embed  $\mathcal{H} \subset \mathcal{H}_+ \oplus \mathcal{H}_-$  where  $\mathcal{H}_\pm = \Gamma(V_\pm, \mathcal{H})$  and the map  $\phi \mapsto (\phi_+, \phi_-)$  comes from the restrictions  $\phi_\pm = \phi|_{V_\pm}$ . To test whether a given pair glues to a section, we can check if  $\phi_+|_{V_+ \cap V_-} - \phi_-|_{V_+ \cap V_-} = 0$ . Setting  $\mathcal{H}' = \Gamma(V_+ \cap V_-, \mathcal{H})$ , we get the exact

sequence

$$\mathcal{H} \rightarrow \mathcal{H}_+ \oplus \mathcal{H}_- \rightarrow \mathcal{H}' \quad (4)$$

**Remark 1.** For the embedding, it actually plays a role what types of sections we use. For continuous sections, the embedding is proper, since the condition for glueing two sections is that they agree on the intersection. If we use  $L^2$  sections, then the embedding is an equality, since as classes any two  $L^2$  sections glue, as the intersection is of measure 0. Finally, if one uses differentiable sections such as  $C^1$ , or  $C^\infty$  sections, then one actually needs to glue over open sets. This slightly changes the definition of  $\mathcal{H}_\pm$ . Namely, choose two neighborhoods  $U_\pm$  of  $V_\pm$  with  $\tau(U_+) = U_-$ , then  $X$  is covered by the two open sets  $U_+$  and  $U_-$ . Now,  $\mathcal{H}_\pm := \Gamma_{C^1, C^\infty}(U_\pm, \mathcal{H})$ . In the usual situation, we can choose the neighborhoods so that they retract onto  $V_\pm$ , so there is no big difference. In practice, physical states should be continuous integrable sections.

The action of  $\Theta$  interchanges the two spaces  $\Theta : \mathcal{H}_\pm \rightarrow \mathcal{H}_\mp$ , that is, it takes on the matrix form

$$\Theta = \begin{pmatrix} 0 & \Theta|_{\mathcal{H}_-} \\ \Theta|_{\mathcal{H}_+} & 0 \end{pmatrix} \quad (5)$$

Since  $\Theta$  respects the first decomposition, we can further decompose  $\mathcal{H}_i \subset \mathcal{H}_{i,+} \oplus \mathcal{H}_{i,-}$  as a block matrix consisting of blocks

$$\Theta_i = \begin{pmatrix} 0 & \Theta|_{\mathcal{H}_{i,-}} \\ \Theta|_{\mathcal{H}_{i,+}} & 0 \end{pmatrix}$$

In  $\mathcal{H}_+ \oplus \mathcal{H}_-$ , we can regard Kramers pairs as above,

$$(\phi, \Theta\phi) = ((\phi_+, \phi_-), ((\Theta\phi)_+, (\Theta\phi)_-)) = ((\phi_+, \phi_-), (\Theta(\phi_-), \Theta(\phi_+)))$$

There are now several choices, indeed there are 4 obvious pairs,

$$\begin{aligned} &((\psi_{2i-1,+}, 0), (0, \Theta\psi_{2i-1,+})) & ((\psi_{2i,+}, 0), (0, \Theta\psi_{2i,+})) \\ &((\Theta\psi_{2i-1,-}, 0), (0, -\psi_{2i-1,-})) & ((\Theta\psi_{2i,-}, 0), (0, -\psi_{2i,-})) \end{aligned}$$

These are not linearly independent though, the relations will be given by the transition functions below. By mixing and matching, this leads to the following choice of two Kramers pairs, whose elements give a local basis,

$$\begin{aligned} (\psi_{I,i}, \psi_{II,i}) &= ((\psi_{2i-1,+}, \Theta\psi_{2i,+}), (-\psi_{2i,+}, \Theta\psi_{2i-1,+})) \\ (\bar{\psi}_{I,i}, \bar{\psi}_{II,i}) &= ((\psi_{2i-1,+}, -\Theta\psi_{2i,+}), (\psi_{2i,+}, \Theta\psi_{2i-1,+})) \end{aligned}$$

The first is the basis of the description of [14] as it is possible to choose  $\psi_{2i}, \psi_{2i-1}$  in such a fashion that they glue to a section over certain subdomains [14, 23], that is on  $X^\tau$ :  $\psi_{I/II,i,+} - \psi_{I/II,i,-} = 0$ . The sections in the second pair do not glue, but rather their difference generates the fiber, that is on  $X^\tau$ :  $(\psi_{I,i,+} - \psi_{I,i,-}, \psi_{II,i,+} - \psi_{II,i,-}) = (\phi_i, \Theta\phi_i)$ . This is a manifestation of Majorana Zero Modes discussed later on. A Kramers pair  $(\psi_{I,i}, \psi_{II,i})$  is also commonly written as  $(\phi_i, \Theta\phi_i)$  if we randomly choose  $\phi_i = \psi_{I,i}$  or  $\phi_i = \psi_{II,i}$ , since there is no a priori ordering between the chiral states  $\psi_{I,i}$  and  $\psi_{II,i}$ .

### 2.1.3 Transition functions

**Lemma 1.** *Define the transition function of the Hilbert subbundle  $\mathcal{H}_i$  by*

$$w^i : X \setminus X^\tau \rightarrow U(2); \quad w_{pq}^i(x) := \langle \psi_p(\tau(x)), \Theta\psi_q(x) \rangle, \quad p, q \in \{2i, 2i-1\} \quad (6)$$

*then the time reversal operator acting on  $\mathcal{H}_i$  is locally represented by  $w^i \circ C$ , where  $C$  is the complex conjugation.*

*Proof.* In terms of the action  $\varsigma$  defined on the space of sections  $\Gamma(X, \mathcal{H}_i)$ ,

$$w_{pq}^i(x) = \langle \psi_q(x), -\Theta\psi_p(\tau(x)) \rangle = \overline{\langle \varsigma(\psi_p)(x), \psi_q(x) \rangle}$$

Since a local section in  $\Gamma(X, \mathcal{H}_i)$  can be written as a Kramers pair  $(\psi_{2i-1}, \psi_{2i})$ , the time reversal operator  $\Theta$  or the action  $\varsigma(\psi) = -\Theta \circ \psi \circ \tau$  is locally represented by  $w^i \circ C$ .  $\square$

The transition function  $w^i$  can be extended to the whole momentum space  $X$ , but it has some conceptual advantage to define it on open subsets excluding the fixed points. In physics, the transition function  $w^i$  is also called the gauge transformation induced by the time reversal symmetry, so that for the subbundle  $\mathcal{H}_i$  the gauge group is  $U(2)$ .

Let us choose an open subset  $O \subset X$ , then the local isomorphism  $\Theta : \mathcal{H}_i|_O \rightarrow \mathcal{H}_i|_{\tau(O)}$  is represented by

$$\Theta : O \times \mathbb{C}^2 \rightarrow \tau(O) \times \mathbb{C}^2, \quad (x, v) \mapsto (\tau(x), w^i(x) \bar{v})$$

Apply  $\Theta$  twice to get back to  $O$ ,

$$(x, v) \mapsto (\tau(x), w^i(x) \bar{v}) \mapsto (x, w^i(\tau(x)) \bar{w}^i(x) v)$$

because of  $\Theta^2 = -1$ , we have

$$w^i(\tau(x))\bar{w}^i(x) = -I_2, \quad \text{i.e.,} \quad [w^i]^T(\tau(x)) = -w^i(x) \quad (7)$$

where  $T$  stands for the transpose of a matrix. In particular,  $w^i$  is skew-symmetric at any fixed point  $x \in X^\tau$ , i.e.,  $[w^i]^T(x) = -w^i(x)$ .

**Example 8.** When  $X = \mathbb{S}^3 = \{(\alpha, \beta) \in \mathbb{C}^2, \text{ s.t. } |\alpha|^2 + |\beta|^2 = 1\}$ , the time reversal transformation is defined by  $\tau(\alpha, \beta) = (\bar{\alpha}, -\beta)$ , and the fixed points are  $(\alpha, \beta) = (\pm 1, 0)$ . In addition, the transition function  $w$  is given by

$$w : \mathbb{S}^3 \rightarrow SU(2); \quad (\alpha, \beta) \mapsto \begin{pmatrix} \beta & \alpha \\ -\bar{\alpha} & \bar{\beta} \end{pmatrix}$$

The total transition function over the Hilbert bundle  $\mathcal{H}$  is defined by the block diagonal matrix  $w = \text{diag}\{w_1, \dots, w_n\}$ , i.e.,  $w : X \rightarrow U(2n)$ . Furthermore, a non-degenerate Quaternionic vector bundle is characterized by the transition function  $w$ .

## 2.2 Quaternionic K-theory

**Definition 5.** For a compact Real space  $(X, \tau)$ , the Quaternionic K-group  $KQ(X, \tau)$  is defined to be the Grothendieck group of finite rank Quaternionic vector bundles  $(E, \chi)$  over  $X$ .

From the previous subsection, we know that the Hilbert bundle of a topological insulator is a finite rank Quaternionic vector bundle over the momentum space, which describes the band structure under the time reversal symmetry. Note that the Quaternionic K-group  $KQ(X, \tau)$  classifies stable isomorphism classes of Quaternionic vector bundles over  $X$ . On a trivial bundle over  $X$ , there is a natural Quaternionic structure acting by  $\tau$  on the base and conjugation on the fibers, hence using the Whitney sum to add a trivial bundle makes perfect sense in the Quaternionic setting and one can take the stable isomorphism classes of Quaternionic bundles.

When the involution  $\tau$  is understood, the Quaternionic K-group  $KQ(X, \tau)$  is denoted simply by  $KQ(X)$ . Similar to the complex K-theory, higher  $KQ$ -groups  $KQ^{-j}(X)$  are defined by suspensions,  $KQ$ -theory is extended onto locally compact spaces, and the reduced Quaternionic K-group  $\widetilde{KQ}(X)$  is defined as the kernel of the restriction map  $i^* : KQ(X) \rightarrow KQ(pt)$ .

The Real K-group  $KR(X, \tau)$  is similarly defined as the Grothendieck group of Real vector bundles  $(E, \iota)$  over  $(X, \tau)$  [2]. There exists a canonical isomorphism  $KQ^*(X) \cong KR^{*-4}(X)$ , so it is convenient to compute  $KQ$ -groups by  $KR$ -groups. Furthermore, the Bott periodicity of  $KQ$ -theory can be derived from that of  $KR$ -theory, i.e.,  $KQ^{8-i}(X) \cong KQ^{-i}(X)$ .

As a convention in  $KR$ -theory,  $\mathbb{R}^{p,q}$  denotes  $\mathbb{R}^p \oplus i\mathbb{R}^q$ , where the canonical involution  $\tau$  on  $\mathbb{R}^{p,q}$  is defined by the complex conjugation so that  $\tau|_{\mathbb{R}^p} = +1$  and  $\tau|_{i\mathbb{R}^q} = -1$ . Similarly,  $\mathbb{S}^{p,q}$  denotes the unit sphere in  $\mathbb{R}^{p,q}$  with the induced involution. In this notation the torus  $\mathbb{T}^d$  and the sphere  $\mathbb{S}^d$  equipped with the time reversal involution given in Examples 3 and 4 can be written as  $\mathbb{T}^d = (\mathbb{S}^{1,1})^d$  and  $\mathbb{S}^d = \mathbb{S}^{1,d}$ .

By the decomposition  $\mathbb{S}^{1,d} = \mathbb{R}^{0,d} \cup \{\infty\}$ , one fixed point of the time reversal symmetry is  $\infty$  and the other is  $0 \in \mathbb{R}^{0,d}$ . Furthermore, one can compute the  $KR$ -groups of spheres based on the above decomposition,

$$KR^{-i}(\mathbb{S}^{1,d}) = KO^{-i}(pt) \oplus KR^{-i}(\mathbb{R}^{0,d}) = KO^{-i}(pt) \oplus KO^{-i+d}(pt)$$

**Example 9.**

$$KQ(\mathbb{S}^{1,2}) = KR^{-4}(\mathbb{S}^{1,2}) = KO^{-4}(pt) \oplus KO^{-2}(pt) = \mathbb{Z} \oplus \mathbb{Z}_2$$

$$KQ(\mathbb{S}^{1,3}) = KR^{-4}(\mathbb{S}^{1,3}) = KO^{-4}(pt) \oplus KO^{-1}(pt) = \mathbb{Z} \oplus \mathbb{Z}_2$$

Similarly, one can decompose  $\mathbb{T}^d = (\mathbb{S}^{1,1})^d$  into fixed points plus involutive Euclidean spaces  $\mathbb{R}^{0,k}$  ( $0 \leq k \leq d$ ), so that the  $KQ$ -groups of  $\mathbb{T}^d$  are computed based on an iterative decomposition using retracts,

$$KQ^{-j}(\mathbb{T}^d) = \oplus_{k=0}^d \binom{d}{k} KSp^{-j+k}(pt) = \oplus_{k=0}^d \binom{d}{k} KO^{4-j+k}(pt)$$

Recall that the  $KSp$ -group  $KSp(Y)$  is the Grothendieck group of quaternionic (or symplectic) vector bundles, where  $Sp$  indicates its structure group is the compact symplectic group  $Sp(n)$ , higher  $KSp$ -groups  $KSp^{-i}(Y)$  can be defined by suspensions.

**Example 10.**

$$KQ(\mathbb{T}^2) = KR^{-4}(\mathbb{T}^2) = KO^{-4}(pt) \oplus KO^{-2}(pt) = \mathbb{Z} \oplus \mathbb{Z}_2$$

$$KQ(\mathbb{T}^3) = KR^{-4}(\mathbb{T}^3) = KO^{-4}(pt) \oplus 3KO^{-2}(pt) \oplus KO^{-1}(pt) = \mathbb{Z} \oplus 4\mathbb{Z}_2$$

Another way to compute the KQ-groups of the torus  $\mathbb{T}^d$  is to use the stable homotopy splitting of the torus into spheres, see [13]. The Baum–Connes isomorphism for the free abelian group  $\mathbb{Z}^d$  provides yet another method to compute the KQ-theory of  $\mathbb{T}^d$ , which will be discussed in the next subsection.

There are several long exact sequences, which we can look at corresponding to the different ways to introduce the  $\mathbb{Z}_2$  invariant. The first is the long exact sequence in KQ-theory corresponding to the “exact sequence” [21][II,4.17]  $Z \dashrightarrow X \dashrightarrow X \setminus Z$  for a closed  $Z$ . Here the dashed arrows indicate that we are looking at locally compact spaces and the morphisms in that category which are defined via their one point compactifications. The sequence reads:

$$\cdots KQ^{-j-1}(Z) \rightarrow KQ^{-j}(X \setminus Z) \rightarrow KQ^{-j}(X) \rightarrow KQ^{-j}(Z) \rightarrow \cdots \quad (8)$$

Recall that there is an isomorphism between KR-theory and complex K-theory given by  $KR^{-i}(Y \times S^{0,1}) \cong K^{-i}(Y)$ , so  $KQ^{-j}(Y \times S^{0,1}) = KR^{4-j}(Y \times S^{0,1}) = K^{4-j}(Y) = K^{-j}(Y)$  by Bott periodicity.

**Lemma 2.** *For regular space, with  $Z = V^+ \cap V^-$ , we have the long exact sequence.*

$$\begin{aligned} \cdots &\rightarrow K^{-j-1}(V_+^o) \rightarrow KQ^{-j-1}(X) \rightarrow KQ^{-j-1}(Z) \\ &\rightarrow K^{-j}(V_+^o) \rightarrow KQ^{-j}(X) \rightarrow KQ^{-j}(Z) \rightarrow \cdots \end{aligned} \quad (9)$$

*Proof.* By assumption  $B$  separates so that  $X \setminus Z = V_+^o \amalg V_-^o = V_+^o \times \mathbb{S}^{0,1}$ .  $\square$

If we are in the case of a weak FKMM space, one can now further decompose  $Z$  iteratively. This explains the effective boundary used in [23].

**Example 11.** In the case of  $\mathbb{T}^2$ , we have  $V_+^o \sim \mathbb{S}^1 \times \mathbb{R}$ ,  $Z = \mathbb{S}^{1,1} \sqcup \mathbb{S}^{1,1}$ ,

$$K(V_+^o) \rightarrow KQ(X) \rightarrow KQ(Z)$$

where  $K(V_+^o) = K(\mathbb{S}^1 \times \mathbb{R}) = K^{-1}(\mathbb{S}^1) = \mathbb{Z} \oplus \mathbb{Z}$ ,  $KQ(\mathbb{T}^2) = \mathbb{Z} \oplus \mathbb{Z}_2$  and  $KQ(\mathbb{S}^{1,1}) = KQ(pt) \oplus KQ^{-1}(pt) = \mathbb{Z}$ . In other words, the above exact sequence gives

$$\mathbb{Z} \oplus \mathbb{Z} \rightarrow \mathbb{Z} \oplus \mathbb{Z}_2 \rightarrow \mathbb{Z} \oplus \mathbb{Z}$$

or equivalently,

$$\mathbb{Z} \rightarrow \mathbb{Z}_2 \rightarrow \mathbb{Z}$$

and this explains the lift to  $\mathbb{Z}$  ( $\tilde{K}^{-1}(\mathbb{S}^1)$ ) of the  $\mathbb{Z}_2$  ( $\widetilde{KQ}(\mathbb{T}^2)$ ) invariant.

In the weak FKMM case, i.e., there is a decomposition  $X = X_+ \amalg X_- \amalg X^\tau$ , this induces a long exact sequence involving different K-theories.

**Lemma 3.** *If  $X$  is of weak FKMM type, then there exists a long exact sequence*

$$\begin{aligned} \cdots &\rightarrow KQ^{-j-1}(X_+ \cup X_-) \rightarrow KQ^{-j-1}(X) \rightarrow KSp^{-j-1}(X^\tau) \\ &\rightarrow KQ^{-j}(X_+ \cup X_-) \rightarrow KQ^{-j}(X) \rightarrow KSp^{-j}(X^\tau) \rightarrow \cdots \end{aligned} \quad (10)$$

Where  $X_+ \cup X_-$  has a free  $\mathbb{Z}_2$  action interchanging the spaces. In case that  $X_+$  and  $X_-$  are in different components of  $X \setminus X^\tau$ , then there exists a long exact sequence

$$\begin{aligned} \cdots &\rightarrow K^{-j-1}(X_+) \rightarrow KQ^{-j-1}(X) \rightarrow KSp^{-j-1}(X^\tau) \\ &\rightarrow K^{-j}(X_+) \rightarrow KQ^{-j}(X) \rightarrow KSp^{-j}(X^\tau) \rightarrow \cdots \end{aligned} \quad (11)$$

*Proof.* Using  $X^\tau \dashrightarrow X \dashrightarrow X \setminus X^\tau$ , we get the first sequence by noticing that when restricting the involution  $\tau$  to the fixed points,  $\tau|_{X^\tau}$  becomes trivial, so  $KQ^{-j}(X^\tau, \tau|_{X^\tau}) = KSp^{-j}(X^\tau)$ . Now under the assumption that  $X_+$  and  $X_-$  are in different components of  $X \setminus X^\tau$ , we have  $X \setminus X^\tau = X_+ \amalg X_- = X_+ \amalg \tau(X_+) = X_+ \times \mathbb{S}^{0,1}$ , it follows that  $KQ^{-j}(X \setminus X^\tau) = KQ^{-j}(X_+ \times \mathbb{S}^{0,1}) \simeq K^{-j}(X_+)$ . □

We can also replace the middle terms by  $KQ^{-j}(X) \simeq KR^{-j+4}(X)$ .

**Example 12.** When  $X = \mathbb{S}^{1,3}$ ,  $X^\tau = \mathbb{S}^{0,1}$  and the open set  $\mathbb{S}^{1,3} \setminus \mathbb{S}^{0,1} = \mathbb{R}^{0,3} \setminus \{0\} = X_+ \cup X_-$ , where  $X_+ \sim 3\mathbb{R} \cup 6\mathbb{R}^2 \cup 4\mathbb{R}^3$ . We extract two parts from the long exact sequence, the first part is

$$KSp^{-6}(\mathbb{S}^{0,1}) \rightarrow K^{-5}(X_+) \rightarrow KQ^{-5}(\mathbb{S}^{1,3}) \rightarrow KSp^{-5}(\mathbb{S}^{0,1})$$

that is,

$$2\mathbb{Z}_2 \rightarrow 3\mathbb{Z} \oplus 4\mathbb{Z} \rightarrow \mathbb{Z}_2 \rightarrow 2\mathbb{Z}_2$$

And the second part is

$$KSp^{-2}(\mathbb{S}^{0,1}) \rightarrow K^{-1}(X_+) \rightarrow KQ^{-1}(\mathbb{S}^{1,3}) \rightarrow KSp^{-1}(\mathbb{S}^{0,1})$$

that is,

$$0 \rightarrow 3\mathbb{Z} \oplus 4\mathbb{Z} \rightarrow \mathbb{Z}_2 \rightarrow 0$$



The second part suggests that the  $\mathbb{Z}_2$  ( $KQ^{-1}(\mathbb{S}^{1,3})$ ) invariant comes from one of the 3d components  $\mathbb{R}^3 \in X_+$  ( $\mathbb{Z} \in 4\mathbb{Z}$ ), which corresponds to a fixed point by Poincaré duality. In addition, the first part tells us that the above  $\mathbb{Z}$  component really has its origin in  $KSp^{-6}(\mathbb{S}^{0,1}) = 2\mathbb{Z}_2$ .

Another sequence is the Mayer–Vietoris sequence for a regular space given by the cover by the fundamental domains  $V_+ \cup V_- = X$ . It is given by:

$$KQ^{-j}(X) \xrightarrow{u} KQ^{-j}(V_+) \oplus KQ^{-j}(V_-) \xrightarrow{v} KQ^{-j}(V_+ \cap V_-) \rightarrow \cdots \quad (12)$$

where  $u(\alpha) = (\alpha|_{V_+}, \alpha|_{V_-})$  and  $v(\alpha_1, \alpha_2) = \alpha_1|_{V_+ \cap V_-} - \alpha_2|_{V_+ \cap V_-}$ . This is the KQ-theory version of (4).

**Example 13.** Here  $X = \mathbb{T}^2$ ,  $V_+ = V_- = C$ , where  $C$  is a cylinder whose boundaries are both  $\mathbb{S}^{1,1}$  and  $Z = \mathbb{S}^{1,1} \amalg \mathbb{S}^{1,1}$ .

Finally there is the relative sequence, for a closed subspace  $Y$  in  $X$

$$KQ^{-j-1}(X, Y) \rightarrow KQ^j(X) \rightarrow KQ^j(Y) \rightarrow KQ^j(X, Y) \quad (13)$$

if one identifies  $KQ^{-n}(X, Y)$  with  $\widetilde{KQ}(S^n(X/Y))$ , where  $S^n$  is the  $n$ -fold suspension, then the first map is induced by the quotient  $q : X \rightarrow X/Y$ .

**Example 14.** Using this for  $\mathbb{T}^2$  and  $\mathbb{S}^{1,1} \vee \mathbb{S}^{1,1}$ , one obtains the collapse map  $q : \mathbb{T}^2 \rightarrow \mathbb{S}^2$  and similarly for  $\mathbb{T}^3$ . This is what is used in [13].

## 2.3 Baum–Connes Isomorphism

In [24], Kitaev mentioned the real Baum–Connes conjecture [9], which is true for the abelian free group  $\Gamma = \mathbb{Z}^d$ , i.e., the translational symmetry of a crystal, so we call it the Baum–Connes isomorphism in this paper. The assembly map was used to understand and calculate the KO-theory of  $\mathbb{T}^d$  in [24]. In this subsection we clarify the Baum–Connes isomorphism in KR-theory.

**Definition 6.** Let  $\Gamma$  be a discrete countable group, the assembly map  $\mu$  is a morphism from the equivariant K-homology of the total space of the classifying bundle  $E\Gamma$  with proper action by  $\Gamma$  to the K-theory of the reduced group  $C^*$ -algebra of  $\Gamma$ , i.e.,

$$\mu(\Gamma) : K_j^\Gamma(E\Gamma) \rightarrow K_j(C_\lambda^*(\Gamma, \mathbb{C}))$$

The classical complex Baum–Connes conjecture states that the assembly index map  $\mu$  is an isomorphism. If  $\Gamma$  is torsion free, then the left hand side is reduced to the ordinary K-homology of the classifying space  $B\Gamma$ , i.e.,  $K_j^\Gamma(E\Gamma) = K_j(B\Gamma)$ .

**Definition 7.** In the real case, the assembly map is similarly defined as

$$\mu_{\mathbb{R}}(\Gamma) : KO_j^\Gamma(E\Gamma) \rightarrow KO_j(C_\lambda^*(\Gamma, \mathbb{R}))$$

The real Baum–Connes conjecture follows from the complex Baum–Connes conjecture, so  $\mu_{\mathbb{R}}(\mathbb{Z}^d)$  is an isomorphism.

If one defines the real function algebra on the Real space  $(X, \tau)$ ,

$$C_0(X, \tau) := \{f \in C_0(X) \mid \overline{f(x)} = f(\tau(x))\}$$

then the KR-theory of  $(X, \tau)$  is identified with the topological K-theory of the above real function algebra [27],

$$KR^{-i}(X, \tau) = KO_i(C_0(X, \tau))$$

By the real assembly map, one has the Baum–Connes isomorphism, sometimes also called the dual Dirac isomorphism, since  $\mathbb{T}^d$  is the classifying space for  $\mathbb{Z}^d$  with universal cover  $\mathbb{R}^d$ .

$$KO_i(\mathbb{T}^d) = KO_i^{\mathbb{Z}^d}(\mathbb{R}^d) \cong KO_i(C^*(\mathbb{Z}^d, \mathbb{R})) = KR^{-i}(\mathbb{T}^d, \tau) \quad (14)$$

By the Poincaré duality, the real K-homology on the left hand side is identified with a KO-group, i.e.,  $KO_i(\mathbb{T}^d) = KO^{d-i}(\mathbb{T}^d)$ . Thus the KQ-groups of  $\mathbb{T}^d$  can be computed by the KO-groups,

$$KQ^{-i}(\mathbb{T}^d) = KR^{-i-4}(\mathbb{T}^d) = KO_{i+4}(\mathbb{T}^d) = KO^{d-i-4}(\mathbb{T}^d) \quad (15)$$

**Example 15.**

$$\begin{aligned} KQ(\mathbb{T}^2, \tau) &= KR^{-4}(\mathbb{T}^2) = KO^{-2}(\mathbb{T}^2) \\ KQ(\mathbb{T}^3, \tau) &= KR^{-4}(\mathbb{T}^3) = KO^{-1}(\mathbb{T}^3) \\ KQ^{-1}(\mathbb{T}^3, \tau) &= KR^{-5}(\mathbb{T}^3) = KO^{-2}(\mathbb{T}^3) \end{aligned}$$

The collapse map  $q : \mathbb{T}^d \rightarrow \mathbb{S}^d$  induces a map between KR-groups  $q^* : KR^{-j}(\mathbb{S}^d) \rightarrow KR^{-j}(\mathbb{T}^d) = KO^{d-j}(\mathbb{T}^d)$ . On the other hand, the inclusion  $i : pt \hookrightarrow \mathbb{T}^d$  induces the restriction map  $i^* : KO^{d-j}(\mathbb{T}^d) \rightarrow KO^{d-j}(pt)$ . The composition of these two maps gives rise to

$$i^* \circ q^* : \widetilde{KR}^{-j}(\mathbb{S}^d) \rightarrow \widetilde{KR}^{-j}(\mathbb{T}^d) \rightarrow KO^{d-j}(pt)$$

so that  $i^* \circ q^* = 1$  is the identity map since  $\widetilde{KR}^{-j}(\mathbb{S}^d) = KO^{d-j}(pt)$ .

### 3 Analytical index

In this section, we will look into the analytic  $KQ$ -homology of Majorana zero modes, which is the dual theory of  $KQ$ -theory. First we will study the geometry of Majorana states by comparing it to  $KR$ -cycles in spin geometry [25]. After that we will give the definition of Majorana zero modes and explain the physical meaning of the topological  $\mathbb{Z}_2$  invariant, i.e., the parity of Majorana zero modes. Finally, we will interpret the topological  $\mathbb{Z}_2$  invariant as a mod 2 analytical index of the effective Hamiltonian.

#### 3.1 KQ-cycle

In order to understand Majorana zero modes in a topological insulator, we compare them to Majorana spinors. In spin geometry, using the framework of  $KR$ -homology, one models Majorana spinors by  $KR$ -cycles. As an analogy, we will give the definition of a  $KQ$ -cycle of a time reversal invariant Majorana state.

**Definition 8.** An unbounded K-cycle for an involutive operator algebra  $(\mathcal{A}, \tau)$  is a triple  $(\mathcal{A}, \mathcal{H}, D)$ , commonly called a spectral triple in noncommutative geometry, where  $\mathcal{H}$  is a Hilbert space, and  $\mathcal{A}$  has a representation on  $\mathcal{H}$  by bounded operators, i.e.,  $\pi : \mathcal{A} \rightarrow B(\mathcal{H})$ .  $D$  is a self-adjoint unbounded operator with compact resolvent such that the commutators  $[D, a]$  are bounded operators for all  $a \in \mathcal{A}$ .

In practice,  $\mathcal{A}$  is always assumed to be a unital pre- $C^*$ -algebra, and  $\tau$  is the anti-linear involution given by the adjoint of operators (the  $*$ -operation). When the representation  $\pi$  is understood, it is skipped from the notation.  $D$  is usually taken as a self-adjoint Dirac operator, and there is a natural action by the real Clifford algebra  $Cl_{p,q}$ .

An unbounded K-cycle  $(\mathcal{A}, \mathcal{H}, D)$  is even if there exists a self-adjoint grading operator  $\gamma$ , i.e.,  $\gamma^* = \gamma$  and  $\gamma^2 = 1$  such that  $D\gamma = -\gamma D$  and  $\gamma a = a\gamma$  for all  $a \in \mathcal{A}$ .

A general real structure on an even K-cycle is defined by an anti-linear isometry  $J$  such that

$$JD = DJ, \quad J^2 = \epsilon, \quad J\gamma = \varepsilon\gamma J \quad (16)$$

where  $\epsilon, \varepsilon = \pm 1$  depending on the dimension  $2k \bmod 8$ . In fact, when  $2k = 0, 6 \bmod 8$ , one has  $\epsilon = 1$  such that  $J^2 = 1$ , and  $J$  is called a real

structure. When  $2k = 2, 4 \bmod 8$ ,  $J^2 = -1$  and  $J$  is called a quaternionic structure. In addition,  $\varepsilon = (-1)^k$  is determined by the grading operator  $\gamma$ .

**Definition 9.** An even  $KR_{2k}$ -cycle (depending on  $2k \bmod 8$ ) is defined as an even unbounded K-cycle equipped with a general real structure, i.e., a quintuple  $(\mathcal{A}, \mathcal{H}, D, \gamma, J)$ , satisfying the relations,

$$JD = DJ, \quad J^2 = \varepsilon, \quad J\gamma = (-1)^k \gamma J$$

where  $J^2 = 1$  if  $2k = 0, 6 \bmod 8$  and  $J^2 = -1$  if  $2k = 2, 4 \bmod 8$ .

By the representation theory of the real Clifford algebra  $Cl_{2k,0}$  [25], when  $2k = 0 \bmod 8$ , it has a unique real pinor representation (i.e., Majorana pinor) and there are two inequivalent real spinor representations (i.e., Majorana–Weyl spinors). When  $2k = 2 \bmod 8$ , it has a unique quaternionic pinor representation (i.e., symplectic Majorana pinor) and there are two inequivalent complex spinor representations (i.e., Majorana–Weyl spinors). When  $2k = 4 \bmod 8$ , it has a unique quaternionic pinor representation (i.e., symplectic Majorana pinor) and there are two inequivalent quaternionic spinor representations (i.e., symplectic Majorana–Weyl spinors). When  $2k = 6 \bmod 8$ , it has a unique real pinor representation (i.e., Majorana pinor) and there are two inequivalent complex spinor representations (i.e., Majorana–Weyl spinors).

**Example 16.** When  $2k = 4 \bmod 8$ , one has symplectic (or quaternionic) Majorana–Weyl spinors modeled by a  $KR_4$ -cycle  $(\mathcal{A}, \mathcal{H}, D, \gamma, J)$  such that

$$JD = DJ, \quad J^2 = -1, \quad J\gamma = \gamma J$$

Similarly, when there is no grading operator, one defines an odd  $KR$ -cycle by a quadruple  $(\mathcal{A}, \mathcal{H}, D, J)$ .

**Definition 10.** An odd  $KR_{2k-1}$ -cycle (for  $2k - 1 \equiv 1, 3, 5, 7 \bmod 8$ ) is defined as a quadruple  $(\mathcal{A}, \mathcal{H}, D, J)$  satisfying the relations,

$$JD = (-1)^k DJ, \quad J^2 = \varepsilon$$

where  $J^2 = 1$  if  $2k - 1 = 1, 7 \bmod 8$  and  $J^2 = -1$  if  $2k - 1 = 3, 5 \bmod 8$ .

The representation theory of the real Clifford algebra in odd dimensions is easier, when  $2k - 1 = 1, 7 \bmod 8$ , there is a unique real spinor representation; when  $2k - 1 = 3, 5 \bmod 8$ , there is a unique quaternionic spinor representation.

**Example 17.** When  $2k - 1 = 1 \bmod 8$ , one has a real spinor modeled by a  $KR_1$ -cycle  $(\mathcal{A}, \mathcal{H}, D, J)$  such that

$$JD = -DJ, \quad J^2 = 1$$

Furthermore, the set of homotopy equivalence classes of  $KR$ -cycles defines the  $KR$ -homology group, for details see [8, 18]. The following example is the classical Dirac geometry modeling (Majorana) spinors in spin geometry [25].

**Example 18.** Let  $M$  be a compact spin manifold of dimension  $2k$ , its Dirac geometry is defined as the unbounded  $K$ -cycle  $(C^\infty(M), L^2(M, \mathcal{S}), \mathcal{D})$ , where  $L^2(M, \mathcal{S})$  is the Hilbert space of spinors and  $\mathcal{D}$  is the Dirac operator. The grading operator  $\gamma$ , or  $c(\gamma)$  for the Clifford multiplication by  $\gamma$ , is defined as usual in an even dimensional Clifford algebra. In addition, the canonical real structure is given by the charge conjugation operator  $C$  of the Clifford algebra. Thus the quintuple  $(C^\infty(M), L^2(M, \mathcal{S}), \mathcal{D}, \gamma, C)$  defines a  $KR_{2k}$ -cycle. In spin geometry, when a spinor  $\psi \in L^2(M, \mathcal{S})$  satisfies  $C\psi = \psi$ , it is called a Majorana spinor, the space of Majorana spinors is denoted by  $L^2(M, \mathcal{S}; C)$ .

Let us now construct a  $KQ$ -cycle based on the geometry of a topological insulator. Let  $H(x)$  be a time reversal invariant Hamiltonian parametrized by  $x \in X$  such that  $\Theta H(x) \Theta^* = H(\tau(x))$ , where  $\Theta$  is the skew-adjoint time reversal operator.  $\Theta$  is an anti-linear isometry such that

$$\Theta H(x) = H(\tau(x)) \Theta, \quad \Theta^2 = -1$$

so  $\Theta$  is a quaternionic structure.

Next we define a grading operator by

$$\gamma := i\Theta$$

which is a self-adjoint operator such that  $\gamma^2 = 1$ . The commutation relation between the grading operation  $\gamma$  and the Hamiltonian is

$$\gamma H(x) = H(\tau(x)) \gamma$$

In general, the Hamiltonian  $H$  of a topological insulator is a linear combination of a Dirac operator and a quadratic correction term, so that  $H(\tau(x)) \neq -H(x)$  and  $\gamma H(x) \neq -H(x) \gamma$ .

**Lemma 4.** *The time reversal operator  $\Theta$  defines a quaternionic structure on the unbounded  $K$ -cycle  $(C^\infty(X), L^2(X, \mathcal{H}), H)$ , it also induces a grading operator  $\gamma = i\Theta$ . The quintuple  $(C^\infty(X), L^2(X, \mathcal{H}), H, \gamma, \Theta)$  defines a generalized  $KR_4$ -cycle over the Real space  $(X, \tau)$  satisfying*

$$\gamma H(x) = H(\tau(x))\gamma, \quad \Theta^2 = -1, \quad \Theta\gamma = \gamma\Theta$$

*which will be called a  $KQ$ -cycle. Let  $\mathcal{H}$  be the even rank Hilbert bundle, such that  $\mathcal{H} = L^2(X, \mathcal{H})$ , as discussed previously.*

The  $KQ$ -cycle constructed above can be regarded as an element of  $KQ$ -homology, so it is expected to be paired with the  $KQ$ -theory to get an index number. It turns out that such pairing does not work for all cases. In fact, there is an alternative construction of a  $KQ$ -cycle based on the geometry of Majorana zero modes, which is the more fundamental.

## 3.2 Majorana zero modes

Before we give the definition of Majorana zero modes, let us first explain what a Majorana state is. Based on Majorana states, we can construct a new  $KQ$ -cycle.

Given a time reversal invariant Hamiltonian  $H$ , we consider its eigenvalue equation, i.e.,  $H(x)\phi(x) = E(x)\phi(x)$  for any eigenstate  $\phi$ . Notice that  $\Theta\phi$  is an orthogonal state (i.e.,  $\langle\phi, \Theta\phi\rangle = 0$ ) with the eigenvalue equation  $H(\tau(x))\Theta\phi(x) = E(\tau(x))\Theta\phi(x)$ . So a Kramers pair  $(\phi, \Theta\phi)$  has the same band, that is given by the flipped eigenvalue functions  $E$  and  $\tau^*E$ , where  $\tau^*E(x) = E(\tau(x))$ . In condensed matter physics, it is called the Kramers' degeneracy theorem, that is, any energy level of a time reversal invariant electronic system is doubly degenerate.

**Lemma 5.** *If we define the effective Hamiltonian  $\tilde{H}$  acting on a Kramers pair  $(\phi, \Theta\phi)$  by*

$$\tilde{H}(x) := \begin{pmatrix} 0 & \Theta H(x) \Theta^* \\ H(x) & 0 \end{pmatrix} \quad (17)$$

*If  $\phi$  is an eigenstate with eigenvalue  $E$  the equation has a matrix form,*

$$\begin{pmatrix} 0 & \Theta H \Theta^* \\ H & 0 \end{pmatrix} \begin{pmatrix} \phi \\ \Theta\phi \end{pmatrix} = \begin{pmatrix} \tau^* E \Theta\phi \\ E \phi \end{pmatrix} \quad (18)$$

In spin geometry, the Dirac operator is decomposed as  $D = \begin{pmatrix} 0 & D_- \\ D_+ & 0 \end{pmatrix}$ , where  $D_+$  (resp.  $D_-$ ) corresponds to the eigenvalue  $+1$  (resp.  $-1$ ) of the grading operator. Based on its eigenvalue equation (18), the effective Hamiltonian  $\tilde{H}$  plays a similar role as the  $\mathbb{Z}_2$ -graded Dirac operator  $D$ . As a result,  $H$  (resp.  $\Theta H \Theta^*$ ) is compared to  $D_+$  (resp.  $D_-$ ), which switches the chiral states in a Kramers pair, i.e.,

$$H : \phi \mapsto \tau^* E \Theta \phi, \quad \Theta H \Theta^* : \Theta \phi \mapsto E \phi$$

In a sense, the chirality of a chiral state can be changed by applying  $\tilde{H}$ .

Define a real structure on the Hilbert bundle  $\mathcal{H}$  by

$$\mathcal{J} := \begin{pmatrix} 0 & \Theta^* \\ \Theta & 0 \end{pmatrix}$$

such that  $\mathcal{J}^* = \mathcal{J}$  and  $\mathcal{J}^2 = 1$ . Since the real structure  $\mathcal{J}$  acts on a local section  $\Phi = (\phi, \Theta \phi)$  by

$$\begin{pmatrix} 0 & \Theta^* \\ \Theta & 0 \end{pmatrix} \begin{pmatrix} \phi \\ \Theta \phi \end{pmatrix} = \begin{pmatrix} \phi \\ \Theta \phi \end{pmatrix} \quad \text{i.e. } \mathcal{J}\Phi = \Phi$$

such local section  $\Phi$  will be defined as a Majorana state.

**Definition 11.** Define a Majorana state as a local section of the Hilbert subbundle  $\mathcal{H}_i$ :  $\Phi_i = (\phi_i, \Theta \phi_i) \in \Gamma(X, \mathcal{H}_i)$ , i.e., a Kramers pair, since it satisfies the real condition  $\mathcal{J}\Phi_i = \Phi_i$  with respect to  $\mathcal{J}$ .

In addition, the commutation relation between the real structure and the effective Hamiltonian is  $\mathcal{J}\tilde{H} = -\tilde{H}\mathcal{J}$ , more explicitly,

$$\begin{pmatrix} 0 & \Theta^* \\ \Theta & 0 \end{pmatrix} \begin{pmatrix} 0 & \Theta H \Theta^* \\ H & 0 \end{pmatrix} \begin{pmatrix} 0 & \Theta^* \\ \Theta & 0 \end{pmatrix} = \begin{pmatrix} 0 & \Theta^* H \Theta^* \\ \Theta^2 H & 0 \end{pmatrix} = \begin{pmatrix} 0 & -\Theta H \Theta^* \\ -H & 0 \end{pmatrix}$$

**Lemma 6.**  $(\mathcal{H}, \mathcal{J}) \rightarrow (X, \tau)$  is a Real Hilbert bundle with quaternionic fibers, and the quadruple  $(C^\infty(X), L^2(X, \mathcal{H}), \tilde{H}, \mathcal{J})$  defines a generalized  $KR_1$ -cycle such that

$$\mathcal{J}\tilde{H} = -\tilde{H}\mathcal{J}, \quad \mathcal{J}^2 = 1$$

A classical Real space is a complex vector space equipped with a real structure, but in our case it is a quaternionic vector space, with a basis given

by  $i, \Theta, i\Theta$ , equipped with a real structure, so we call it a *generalized  $KR_1$ -cycle*, or a  $KQ_1$ -cycle. In order to get an index number, a  $KQ_1$ -cycle is expected to be paired with the  $KQ^{-1}$ -group.

Now we can talk about zero modes of Majorana states, which will be called Majorana zero modes. In a Majorana state  $\Phi = (\phi, \Theta\phi)$ ,  $\phi$  and  $\Theta\phi$  are orthogonal, hence linearly independent. In particular, at their intersection, i.e.,  $\Theta\phi(x) = \phi(x)$ , for a fixed point  $x \in X^\tau$ , they must have zero energies at that fixed point, i.e.,  $\phi(x) = 0 = \Theta\phi(x)$ .

**Definition 12.** A Majorana zero mode is defined as a local Majorana state  $\Phi_0 = (\phi_0, \Theta\phi_0)$  such that  $\phi_0(x) = \Theta\phi_0(x) = 0$  for some fixed point  $x \in X^\tau$ .

By definition, a Majorana zero mode can be found only in a small neighborhood of a fixed point. The local geometric picture of a Majorana zero mode is given by a conical singularity, for example a cone  $V(x^2 + y^2 - z^2)$  in 3d, at the intersection, the cone is called a Dirac cone and the intersection is called a Dirac point by physicists.

**Definition 13.** The topological  $\mathbb{Z}_2$  invariant of a time reversal invariant topological insulator is defined as the parity of Majorana zero modes.

This definition gives the physical meaning of the topological  $\mathbb{Z}_2$  invariant, we will interpret it as a mod 2 analytical index in the next subsection.

Around a fixed point, a chiral state  $\phi$  and its mirror partner  $\Theta\phi$  may intersect with each other. In a Majorana zero mode  $\Phi_0 = (\phi_0, \Theta\phi_0)$ , a chiral zero mode  $\phi_0$  or  $\Theta\phi_0$  will change the sign of its eigenvalue after going across each other. Let us consider the spectral flow of a chiral zero mode, the parity of Majorana zero modes can be computed as a mod 2 spectral flow.

Fix a chiral zero mode  $\phi_0$  or  $\Theta\phi_0$  in a Majorana zero mode, if its sign changes from negative to positive when passing through a fixed point, then the spectral flow of the chosen chiral zero mode will increase by 1. On the other hand, if its sign changes in the negative direction, the spectral flow will decrease by 1. So around a fixed point, the spectral flow of a chiral zero mode could change by  $-1, 0$  or  $1$ .

However, there is no way to tell  $\phi$  and  $\Theta\phi$  apart based on the time reversal symmetry since they are mirror images of each other. Time reversal symmetry does not determine whether a chiral state  $\phi$  or  $\Theta\phi$  is left-moving or right-moving, but only reverses the chirality, that is, interchanges between left-moving and right-moving. As a consequence, if we pick a chiral zero



mode  $\phi_0$  or  $\Theta\phi_0$  around a fixed point, the increase or decrease of the spectral flow of the chosen chiral zero mode at that fixed point by 1 is expected to be equivalent. So the existence of a Majorana zero mode can be counted by either adding or subtracting 1 to the spectral flow.

**Theorem 1.** *The topological  $\mathbb{Z}_2$  invariant can be computed by the mod 2 spectral flow of the Hamiltonian  $H$ .*

*Proof.* Around a fixed point, if we can find a Majorana zero mode, then we use the spectral flow of a chiral zero mode to count that Majorana zero mode. Running through all the fixed points, we count all Majorana zero modes by adding those spectral flows together, which is an integer between  $-k_0$  and  $k_0$  where  $k_0$  is the number of fixed points. So the parity of Majorana zero modes is the cumulative spectral flow of chiral zero modes modulo 2, since Majorana zero modes are local sections of the Hilbert bundle.

The Hamiltonian  $H$  is a self-adjoint Fredholm operator parametrized by  $x \in X$ , its eigenstate with zero energy gives a chiral zero mode at a fixed point. So the spectral flow of the Hamiltonian counts all the sign changes of those local chiral zero modes running over all the fixed points. Therefore, the mod 2 spectral flow of the Hamiltonian computes the topological  $\mathbb{Z}_2$  invariant. It is different from the spectral flow of a pair of self-adjoint Fredholm operators, which computes the integral Fredholm index.  $\square$

**Remark 2.** Another way to understand  $\tilde{H}$  is that this is the local perturbation around the set of fixed points of the family of Hamiltonians. This was used in [23] in order to strictly define the Kramers pair  $(\psi_I, \psi_{II})$ . Moreover trivializing the bundle in a neighborhood of a fixed point using a Kramers pair  $(\phi, \Theta\phi)$  we can write  $(\psi_I, \psi_{II}) = (\psi_I - \phi, \psi_{II} - \Theta\phi) + (\phi, \Theta\phi)$ , where now the first summand is a Majorana zero mode. This ties in with the description in §2.1.2. It also gives the perturbation of  $H(x + \epsilon) = H(x) + \epsilon\tilde{H}$  that is typical for Dirac points.

### 3.3 Mod 2 index

Atiyah and Singer introduced a mod 2 analytical index of real skew-adjoint elliptic operators in [5],

$$\text{ind}_2(P) := \dim \ker P \mod 2$$

In this subsection, we will explain that the topological  $\mathbb{Z}_2$  invariant can be interpreted as the mod 2 analytical index of the effective Hamiltonian  $\tilde{H}$  (17). If the topological  $\mathbb{Z}_2$  invariant is an analytical index, then it is expected to live in some K-group. Let us look at the effective Hamiltonian again, and relate it to the classifying spaces of KR-theory.

From the previous subsection, we know the effective Hamiltonian of a Majorana zero mode is given by  $\tilde{H} = \begin{pmatrix} 0 & \Theta H \Theta^* \\ H & 0 \end{pmatrix}$ , where  $\Theta H(x) \Theta^* = H(\tau(x))$  and  $H^* = H$ .

**Lemma 7.** *The effective Hamiltonian  $\tilde{H}$  is an almost skew-adjoint operator.*

*Proof.* In general, the time reversal invariant Hamiltonian  $H$  of a topological insulator is a linear combination of a Dirac operator and a quadratic correction term. Let us look at the adjoint of  $\tilde{H}$ ,

$$\tilde{H}^* = \begin{pmatrix} 0 & H^* \\ \Theta H^* \Theta^* & 0 \end{pmatrix} = \begin{pmatrix} 0 & H \\ \Theta H \Theta^* & 0 \end{pmatrix}$$

In the above, if the Hamiltonian  $H$  is replaced by a Dirac operator  $D$ , which has the natural property  $\Theta D \Theta^* = -D$ , then  $\tilde{H}$  will become a skew-adjoint Fredholm operator, i.e.,  $\tilde{H}^* = -\tilde{H}$ . After adding a quadratic correction term into the Hamiltonian  $H$ , the effective Hamiltonian  $\tilde{H}$  still belongs to the same homotopy class since  $H$  can be viewed as a continuous deformation of the Dirac operator  $D$ . In other words,  $\tilde{H}$  is a perturbation of a skew-adjoint operator.  $\square$

**Theorem 2.** *The topological  $\mathbb{Z}_2$  invariant is the mod 2 analytical index of the effective Hamiltonian  $\tilde{H}$ ,*

$$\nu = \text{ind}_2(\tilde{H}) \tag{19}$$

*Proof.* Since  $\tilde{H}$  is almost skew-adjoint and the analytical index map is homotopy invariant, the mod 2 index of  $\tilde{H}$  is well defined,

$$\text{ind}_2(\tilde{H}) = \dim \ker \tilde{H} \pmod{2}$$

Suppose  $\Psi = (\psi, \Theta\psi) \in \ker \tilde{H}$ , i.e.,

$$\begin{pmatrix} 0 & \Theta H \Theta^* \\ H & 0 \end{pmatrix} \begin{pmatrix} \psi \\ \Theta\psi \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

then  $H(x)\psi(x) = 0$  and  $H(\tau(x))\Theta\psi(x) = 0$ . It only happens when  $\Psi$  is a Majorana zero mode around a fixed point. Thus the mod 2 index  $ind_2(\tilde{H})$  is nothing but the parity of Majorana zero modes.  $\square$

In [4], the classifying spaces of KR-groups are constructed by different classes of Fredholm operators. In [16], the classes of Fredholm operators are equivalently defined by different symmetries of general topological insulators. In the next paragraph, we identify the above analytical index as an element in  $KO^{-2}(pt)$  following [4].

Let  $\mathcal{F}(\mathcal{H}, J)$  denote the space of Fredholm operators on a Real Hilbert space  $(\mathcal{H}, J)$ , where  $J$  is a real structure such that  $J^2 = 1$ . In addition, let  $\hat{\mathcal{F}}(\mathcal{H}, J)$  denote the space of skew-adjoint Fredholm operators, so  $\hat{\mathcal{F}}(\mathcal{H}, J)$  is a classifying space of  $KR^{-1}$ , i.e.,  $KR^{-1}(X) = [X, \hat{\mathcal{F}}(\mathcal{H}, J)]$  for a compact Real space  $(X, \tau)$ . In our case, the effective Hamiltonian  $\tilde{H}$  is an almost skew-adjoint Fredholm operator acting on the Real Hilbert space  $(L^2(X, \mathcal{H}), \mathcal{J})$ , so the analytical index belongs to  $KO^{-2}(pt)$ ,

$$ind_a : \hat{\mathcal{F}}(L^2(X, \mathcal{H}), \mathcal{J}) \rightarrow KO^{-2}(pt) = \mathbb{Z}_2 \quad (20)$$

Note that if  $\mathcal{H}$  is a complex Hilbert space, then the analytical index lives in  $KO^{-1}(pt)$ . However, in our case  $L^2(X, \mathcal{H})$  is a quaternionic Hilbert space since a local section is given by  $(\phi, \Theta\phi) \in \mathbb{C} \oplus \Theta\mathbb{C}$ , so  $ind_a(\tilde{H}) \in KO^{-2}(pt)$ .

## 4 Topological index

The Atiyah–Singer index theorem teaches us that the analytical index is equal to the topological index. In this section, we will compute the mod 2 analytical index, i.e., the topological  $\mathbb{Z}_2$  invariant, by topological index formulae. In even dimensions, the topological index is the Chern character of the projection representing the Hilbert bundle. While in odd dimensions, the topological index is the odd Chern character of the gauge transformation characterizing the Hilbert bundle. In this paper, we only give examples in 2d and 3d, which are cases of interest for condensed matter physics.

### 4.1 Topological index

Given a skew-adjoint operator  $P$  with the symbol class  $[\sigma(P)] \in KR^{-2}(TX)$ , the topological index of  $[\sigma(P)]$  was constructed by Atiyah [3],

$$ind_t : KR^{-2}(TX) \rightarrow KO^{-2}(pt) = \mathbb{Z}_2 \quad (21)$$

For a  $d$ -dimensional involutive space  $(X, \tau)$ , the Thom isomorphism in  $KR$ -theory is given by

$$KR^{-j}(X) \cong KR^{d-j}(TX) \quad (22)$$

**Example 19.** When  $X = \mathbb{T}^2$ , the topological index can be understood as a map from  $KQ(\mathbb{T}^2)$  to  $\mathbb{Z}_2$  since the Thom isomorphism identifies  $KQ(\mathbb{T}^2)$  with  $KR^{-2}(T\mathbb{T}^2)$ ,

$$ind_t : KQ(\mathbb{T}^2) = KR^{-4}(\mathbb{T}^2) \cong KR^{-2}(T\mathbb{T}^2) \rightarrow KO^{-2}(pt)$$

**Example 20.** When  $X = \mathbb{T}^3$ , the topological index can be understood as a map from  $KQ^{-1}(\mathbb{T}^3)$  to  $\mathbb{Z}_2$ ,

$$ind_t : KQ^{-1}(\mathbb{T}^3) = KR^{-5}(\mathbb{T}^3) \cong KR^{-2}(T\mathbb{T}^3) \rightarrow KO^{-2}(pt)$$

The topological index can be explicitly computed by the Chern character, which is a map from K-theory to de-Rham cohomology by the classical Chern–Weil theory. In a modern language, the topological index can be obtained by the pairing between KQ-homology and KQ-theory.

For the Example 20,  $\widetilde{KQ}(\mathbb{T}^3) \cong 3KO^{-2}(pt) \oplus KO^{-1}(pt)$  and  $\widetilde{KQ}^{-1}(\mathbb{T}^3) \cong 3KO^{-4}(pt) \oplus KO^{-2}(pt)$  both contain the information about the topological  $\mathbb{Z}_2$  invariant. But the topological index map picks  $KO^{-2}$  as the right K-theory, which matches with the result on the KQ-cycle of Majorana zero modes. In other words, this index number is obtained from the pairing between an element in the  $KO^{-2}$ -group and a  $KQ_1$ -cycle.

## 4.2 2d case

For the 2d momentum spaces  $X = \mathbb{S}^2$  or  $\mathbb{T}^2$ , choose a projection  $p$  representing the generator of  $\widetilde{KQ}(X) \cong \mathbb{Z}_2$ , corresponding to a Quaternionic vector bundle  $(\mathcal{H}, \Theta) \rightarrow (X, \tau)$ . Without loss of generality, we assume the Hilbert bundle  $\mathcal{H}$  is of rank 2, since  $\widetilde{KQ}(X)$  only contains information about the first Chern class for a 2d  $X$ . The topological index can be computed by the Chern character of  $p$ ,

$$ind(p) = \frac{1}{2\pi} \int_X tr(pdpdp) \quad (23)$$

which is also known as the first Chern number  $c_1$ .

**Example 21.** If we define the 2d sphere in real coordinates

$$\mathbb{S}^2 = \{(x, y, z) \in \mathbb{R}^3 \mid x^2 + y^2 + z^2 = 1\}$$

then the Hopf bundle over  $\mathbb{S}^2$  can be represented by the projection  $p \in C(S^2)$  or the unitary  $u = 2p - 1$ ,

$$p = \frac{1}{2} \begin{pmatrix} 1+z & x+iy \\ x-iy & 1-z \end{pmatrix}, \quad u = \begin{pmatrix} z & x+iy \\ x-iy & -z \end{pmatrix}$$

So the first Chern character  $Ch_1(p) = tr(pdpdp)$  is the standard volume form on  $\mathbb{S}^2$ ,

$$tr(pdpdp) = \frac{-i}{2}(xdydz - ydxdz + zdxdy)$$

The time reversal transformation on  $\mathbb{S}^2$  is  $\tau : (x, y, z) \mapsto (x, -y, -z)$ , and the first Chern character does not change under  $\tau$ , i.e.,  $Ch_1(p) = Ch_1(\tau^*(p))$ .

**Theorem 3.** *The first Chern class of the Hilbert bundle  $\pi : \mathcal{H} \rightarrow X$  is a 2 torsion, i.e.,*

$$2c_1(\mathcal{H}) = 0, \quad c_1(\mathcal{H}) \in H^2(X, \mathbb{Z}), \quad (24)$$

*Proof.* Consider the pullback bundle  $\tau^*\mathcal{H}$  over  $X$ ,

$$\begin{array}{ccc} \tau^*\mathcal{H} & \xrightarrow{\mathcal{J}} & \mathcal{H} \\ \downarrow & & \downarrow \\ X & \xrightarrow{\tau} & X \end{array}$$

Fix a point  $x \in X$  and a small neighborhood  $O$  around  $x$ , let us look at the point  $\tau(x) \in X$ , in its neighborhood  $\tau(O)$  a local section  $\Phi \in \Gamma(X, \mathcal{H})$  is given by a Majorana state  $\Phi = (\phi, \Theta\phi)$ . Recall that we defined a pullback action  $\iota(\phi) = -\Theta \circ \phi \circ \tau$ , apply  $\iota \otimes I_2$  to a Majorana state  $\Phi$  over  $\tau(x)$ ,

$$\begin{pmatrix} \iota & 0 \\ 0 & \iota \end{pmatrix} \begin{pmatrix} \phi(\tau(x)) \\ \Theta\phi(\tau(x)) \end{pmatrix} = \begin{pmatrix} -\Theta\phi(\tau^2(x)) \\ -\Theta^2\phi(\tau^2(x)) \end{pmatrix} = \begin{pmatrix} -\Theta\phi(x) \\ \phi(x) \end{pmatrix}$$

So the pullback bundle  $\tau^*\mathcal{H}$  has a local section  $(-\Theta\phi, \phi)$  corresponding to the Majorana state  $\Phi = (\phi, \Theta\phi)$ . Since the time reversal operator  $\Theta$  is an anti-unitary operator, we have the conclusion that the pullback bundle is isomorphic to the conjugate bundle, i.e.,  $\tau^*\mathcal{H} \cong \overline{\mathcal{H}}$ , which is compatible with the time reversal transformation  $\tau$  being orientation-reversing.

On the other hand, the pullback bundle  $\tau^*\mathcal{H}$  can be identified with  $\mathcal{J}(\mathcal{H})$ , since  $\mathcal{J}$  is an involutive bundle isomorphism. In addition,  $\mathcal{J}$  is a real structure such that  $\mathcal{J}\Phi = \Phi$  for any Majorana state  $\Phi = (\phi, \Theta\phi)$ , so  $\mathcal{J}(\mathcal{H}) \cong \mathcal{H}$ . In sum, we have the bundle isomorphism,

$$\mathcal{H} \cong \mathcal{J}(\mathcal{H}) \cong \tau^*\mathcal{H} \cong \overline{\mathcal{H}}$$

Therefore, the first Chern class of the Hilbert bundle  $\mathcal{H}$  is a 2 torsion,

$$c_1(\mathcal{H}) = c_1(\overline{\mathcal{H}}) = -c_1(\mathcal{H}), \quad i.e., \quad 2c_1(\mathcal{H}) = 0$$

□

In other words, the topological index  $ind(p)$  is naturally  $\mathbb{Z}_2$ -valued, which is exactly reflected by  $\widehat{KQ}(X) = \mathbb{Z}_2$  for  $X = \mathbb{S}^2$  or  $\mathbb{T}^2$ .

As a special case, if the Hilbert bundle can be decomposed into two line bundles

$$\mathcal{H} = \mathcal{L} \oplus \tau^*\mathcal{L} \cong \mathcal{L} \oplus \overline{\mathcal{L}}$$

then the first Chern class of  $\mathcal{H}$  is zero,

$$c_1(\mathcal{H}) = c_1(L) + c_1(\overline{\mathcal{L}}) = c_1(L) - c_1(\mathcal{L}) = 0$$

We have to point out that such decomposition of the Hilbert bundle is not always valid, which is different from a spin bundle.

### 4.3 3d case

For the 3d momentum spaces  $X = \mathbb{T}^3$  or  $\mathbb{S}^3$ , we assume the rank of the Hilbert bundle  $\pi : \mathcal{H} \rightarrow X$  is 2, i.e.,  $rank(\mathcal{H}) = 2$ . Recall that the transition function  $w$  in eq.(6) defines a map  $w : X \rightarrow U(2)$ , so the structure or gauge group is  $U(2)$ . If, in addition, the Majorana states  $\Phi$  are assumed to be normalized such that  $\langle \Phi, \Phi \rangle = 1$ , then the gauge group  $U(2)$  is reduced to  $SU(2) \simeq Sp(1)$ .

The involutions of the Hilbert bundle  $(\mathcal{H}, \mathcal{J}) \rightarrow (X, \tau)$  induces an involution on the structure group. Define  $\sigma : U(2) \rightarrow U(2)$  by  $\sigma(g) \mapsto -g^{-1}$  so that  $\sigma^2 = 1$ . One can check that  $w \circ \tau = \sigma \circ w$ , so that with this involution on the gauge group, the transition function  $w$  defines an equivariant map between the Real space and the involutive group

$$w : (X, \tau) \rightarrow (U(2), \sigma)$$

Furthermore,  $w$  gives rise to the generator  $[w]$  of  $\widetilde{KQ}^{-1}(X) \simeq \mathbb{Z}_2$  for  $X = \mathbb{S}^3$  or  $\mathbb{T}^3$ . In physical terms, we consider the gauge theory of a topological insulator, and  $w$  is the gauge transformation induced by the time reversal symmetry characterizing the band structure.

The odd Chern character of a map  $g$  on  $X$  with values in  $U(n)$  is defined by [15],

$$Ch(g) := \sum_{k=0}^{\infty} (-1)^k \frac{k!}{(2k+1)!} tr[(g^{-1}dg)^{2k+1}] \quad (25)$$

which is a closed form of odd degree. The topological index in odd dimensions can be computed by the odd index theorem [7], when the Dirac or A-roof genus  $\hat{A}(X) = 1$ ,

$$ind(g) = \frac{1}{4\pi^2} \int_X Ch_3(g) = \frac{1}{4\pi^2} \int_X tr(g^{-1}dg)^3 \quad (26)$$

The right hand side of the above formula is the winding number or degree of  $g$ , that is, the degree of  $g$  computes the spectral flow  $sf(H, g^{-1}Hg)$  [15].

**Proposition 1.** *The topological index of the specific gauge transformation  $w$  induced by the time reversal symmetry, i.e.,  $ind(w)$ , is naturally  $\mathbb{Z}_2$ -valued.*

*Proof.* Using the compatibility condition between the transition function  $w$  and the time reversal transformation  $\tau$ , i.e.,  $\tau^*w = w \circ \tau = \sigma(w) = -w^{-1}$ , we have

$$\begin{aligned} \int_X tr(w^{-1}dw)^3 &= \int_X tr[\tau^*(w^{-1})d(\tau^*w)]^3 \\ &= \int_X tr[(-w)d(-w^{-1})]^3 \\ &= \int_X tr(wdw^{-1})^3 \end{aligned}$$

In general,  $\int_X tr(g^{-1}dg)^3 \neq \int_X tr(gdg^{-1})^3$  since they describe different chiral currents in the opposite direction based on non-abelian bosonization [32]. When the equality holds, the winding number of  $g$  equals that of  $g^{-1}$ , in particular,  $+1$  and  $-1$  can be identified. In other words, the topological index of  $w$  is a mod 2 degree, i.e.,  $ind(w) = deg_2(w)$ . □

The odd index theorem gives one way to compute the topological  $\mathbb{Z}_2$  invariant in odd dimensions, which is also called the Wess–Zumino–Witten (WZW) term in physics. The WZW topological term is an action functional of gauge transformations, if we further consider the effective fermionic field

theory of a topological insulator, it will give rise to a Pfaffian formalism of the topological  $\mathbb{Z}_2$  invariant, which is also called the Kane–Mele invariant by physicists. We will prove the equivalence between these two formalisms of the topological  $\mathbb{Z}_2$  invariant in 3d.

First let us give the definition of the Kane–Mele invariant [19], which works in all dimensions. Recall that at any fixed point  $x \in X^\tau$ , the transition function  $w$  from eq.(6) is a skew-symmetric matrix, i.e.,  $w^T(x) = -w(x)$ , where  $T$  is the transpose of a matrix. So it makes sense to take the Pfaffian of  $w$  at any fixed point  $x \in X^\tau$ , denoted by  $pf[w(x)]$ . Compared with the square root of the determinant of  $w$  at  $x \in X^\tau$ , i.e.,  $\sqrt{\det[w(x)]}$ , the Kane–Mele invariant is defined as the product of the signs of Pfaffians. Recall that the relation between the Pfaffian and determinant function is  $pf^2(A) = \det(A)$  for a skew-symmetric matrix  $A$ , so that  $pf(A) = \pm\sqrt{\det(A)}$ .

**Definition 14.** Assume the set of fixed points  $X^\tau$  is finite, the Kane–Mele invariant of a topological insulator is defined by

$$\nu = \prod_{x_i \in X^\tau} \text{sgn}(pf[w(x_i)]) = \prod_{x_i \in X^\tau} \frac{pf[w(x_i)]}{\sqrt{\det[w(x_i)]}} \quad (27)$$

In principle, the odd  $K^{-1}$ -group can be computed based on the determinant function  $\det$ , and the odd  $KQ^{-1}$ -group can be computed based on the Pfaffian function  $pf$ .

Let us start with the identity  $\ln \det(A) = \text{tr} \ln(A)$  for a square matrix  $A$ , when  $A$  is skew-symmetric, it becomes  $2 \ln pf(A) = \text{tr} \ln(A)$ . The transition function  $w$  is viewed as a matrix parametrized by a 3d momentum space  $w : (X, \tau) \rightarrow (U(2), \sigma)$ , we consider the variation of  $\ln \det(w)$  with respect to the local coordinates of  $X$ .

**Lemma 8.** *The integral form of the variation of  $\ln \det(w)$  equals the WZW topological term,*

$$\int_X d \ln \det(w) = -\frac{1}{4\pi^2} \int_X \text{tr}(w^{-1}dw)^3 \quad (28)$$

*Proof.* Suppose an invertible matrix  $A(x, y, z)$  depends on variables  $x, y, z$ , we consider the third partial derivative of  $\ln \det(A)$  with respect to  $x, y$  and  $z$ . The first partial derivative is well-known,

$$\frac{\partial \ln \det A}{\partial x} = \frac{\partial \text{tr} \ln A}{\partial x} = \text{tr}(A^{-1} \frac{\partial A}{\partial x})$$



The second partial derivative is

$$\begin{aligned}\frac{\partial^2 \ln \det A}{\partial x \partial y} &= \text{tr}(A^{-1} \frac{\partial^2 A}{\partial x \partial y}) + \text{tr}(\frac{\partial A^{-1}}{\partial y} \frac{\partial A}{\partial x}) \\ &= \text{tr}(A^{-1} \frac{\partial^2 A}{\partial x \partial y}) - \text{tr}(A^{-1} \frac{\partial A}{\partial y} A^{-1} \frac{\partial A}{\partial x})\end{aligned}$$

since  $\frac{\partial A^{-1}}{\partial y} A + A^{-1} \frac{\partial A}{\partial y} = 0$  based on  $A^{-1} A = I$ , i.e.,  $\frac{\partial A^{-1}}{\partial y} = -A^{-1} \frac{\partial A}{\partial y} A^{-1}$ . The third partial derivative is

$$\begin{aligned}\frac{\partial^3 \ln \det A}{\partial x \partial y \partial z} &= \text{tr}(A^{-1} \frac{\partial^3 A}{\partial x \partial y \partial z}) + \text{tr}(\frac{\partial A^{-1}}{\partial z} \frac{\partial^2 A}{\partial x \partial y}) \\ &\quad - \text{tr}(\frac{\partial A^{-1}}{\partial z} \frac{\partial A}{\partial y} A^{-1} \frac{\partial A}{\partial x}) - \text{tr}(A^{-1} \frac{\partial^2 A}{\partial y \partial z} A^{-1} \frac{\partial A}{\partial x}) \\ &\quad - \text{tr}(A^{-1} \frac{\partial A}{\partial y} \frac{\partial A^{-1}}{\partial z} \frac{\partial A}{\partial x}) - \text{tr}(A^{-1} \frac{\partial A}{\partial y} A^{-1} \frac{\partial^2 A}{\partial x \partial z}) \\ &= \text{tr}(\frac{\partial \ln A}{\partial x} \frac{\partial \ln A}{\partial y} \frac{\partial \ln A}{\partial z}) + \text{tr}(\frac{\partial \ln A}{\partial x} \frac{\partial \ln A}{\partial z} \frac{\partial \ln A}{\partial y}) + \text{tr}(A^{-1} \frac{\partial^3 A}{\partial x \partial y \partial z}) \\ &\quad + \text{tr}(\frac{\partial A^{-1}}{\partial x} \frac{\partial^2 A}{\partial y \partial z}) + \text{tr}(\frac{\partial^2 A}{\partial x \partial z} \frac{\partial A^{-1}}{\partial y}) + \text{tr}(\frac{\partial^2 A}{\partial x \partial y} \frac{\partial A^{-1}}{\partial z})\end{aligned}$$

so the differential of  $\ln \det A$  is

$$\begin{aligned}d \ln \det A &= [\text{tr}(\frac{\partial \ln A}{\partial x} \frac{\partial \ln A}{\partial y} \frac{\partial \ln A}{\partial z}) + \text{tr}(\frac{\partial \ln A}{\partial x} \frac{\partial \ln A}{\partial z} \frac{\partial \ln A}{\partial y}) + \text{tr}(A^{-1} \frac{\partial^3 A}{\partial x \partial y \partial z}) \\ &\quad + \text{tr}(\frac{\partial A^{-1}}{\partial x} \frac{\partial^2 A}{\partial y \partial z}) + \text{tr}(\frac{\partial^2 A}{\partial x \partial z} \frac{\partial A^{-1}}{\partial y}) + \text{tr}(\frac{\partial^2 A}{\partial x \partial y} \frac{\partial A^{-1}}{\partial z})] dx dy dz \\ &= [\text{tr}(\frac{\partial \ln A}{\partial x} \frac{\partial \ln A}{\partial y} \frac{\partial \ln A}{\partial z}) + \text{tr}(A^{-1} \frac{\partial^3 A}{\partial x \partial y \partial z}) \\ &\quad + \text{tr}(\frac{\partial A^{-1}}{\partial x} \frac{\partial^2 A}{\partial y \partial z}) + \text{tr}(\frac{\partial^2 A}{\partial x \partial y} \frac{\partial A^{-1}}{\partial z})] dx dy dz \\ &\quad - [\text{tr}(\frac{\partial \ln A}{\partial x} \frac{\partial \ln A}{\partial z} \frac{\partial \ln A}{\partial y}) + \text{tr}(\frac{\partial^2 A}{\partial x \partial z} \frac{\partial A^{-1}}{\partial y})] dx dz dy\end{aligned}$$

If we change the order of the variables  $x, y$  and  $z$ , we similarly get

$$\begin{aligned}d \ln \det A &= [\text{tr}(\frac{\partial \ln A}{\partial y} \frac{\partial \ln A}{\partial x} \frac{\partial \ln A}{\partial z}) + \text{tr}(A^{-1} \frac{\partial^3 A}{\partial y \partial x \partial z}) \\ &\quad + \text{tr}(\frac{\partial A^{-1}}{\partial y} \frac{\partial^2 A}{\partial x \partial z}) + \text{tr}(\frac{\partial^2 A}{\partial y \partial x} \frac{\partial A^{-1}}{\partial z})] dy dx dz \\ &\quad - [\text{tr}(\frac{\partial \ln A}{\partial y} \frac{\partial \ln A}{\partial z} \frac{\partial \ln A}{\partial x}) + \text{tr}(\frac{\partial^2 A}{\partial y \partial z} \frac{\partial A^{-1}}{\partial x})] dy dz dx\end{aligned}$$

and

$$\begin{aligned}d \ln \det A &= [\text{tr}(\frac{\partial \ln A}{\partial z} \frac{\partial \ln A}{\partial y} \frac{\partial \ln A}{\partial x}) + \text{tr}(A^{-1} \frac{\partial^3 A}{\partial z \partial y \partial x}) \\ &\quad + \text{tr}(\frac{\partial A^{-1}}{\partial z} \frac{\partial^2 A}{\partial y \partial x}) + \text{tr}(\frac{\partial^2 A}{\partial z \partial y} \frac{\partial A^{-1}}{\partial x})] dz dy dx \\ &\quad - [\text{tr}(\frac{\partial \ln A}{\partial z} \frac{\partial \ln A}{\partial x} \frac{\partial \ln A}{\partial y}) + \text{tr}(\frac{\partial^2 A}{\partial z \partial x} \frac{\partial A^{-1}}{\partial y})] dz dx dy\end{aligned}$$

Combine them together, we have

$$\begin{aligned}-d \ln \det A &= \text{tr}(A^{-1} dA)^3 + 3[\text{tr}(A^{-1} \frac{\partial^3 A}{\partial x \partial y \partial z}) + \text{tr}(\frac{\partial A^{-1}}{\partial x} \frac{\partial^2 A}{\partial y \partial z}) \\ &\quad + \text{tr}(\frac{\partial^2 A}{\partial x \partial z} \frac{\partial A^{-1}}{\partial y}) + \text{tr}(\frac{\partial^2 A}{\partial x \partial y} \frac{\partial A^{-1}}{\partial z})] dx dy dz\end{aligned}$$

where  $\text{tr}(A^{-1}dA)^3 = \sum_{(i,j,k) \in S^3} \epsilon_{ijk} \text{tr}(d_i \ln A d_j \ln A d_k \ln A) dx_i dx_j dx_k$ .

Now we replace  $A$  by  $w$  and take the integral,

$$\begin{aligned} - \int_X d \ln \det w = & \int_X \text{tr}(w^{-1}dw)^3 + 3 \int_X [\text{tr}(w^{-1} \frac{\partial^3 w}{\partial x \partial y \partial z}) + \text{tr}(\frac{\partial w^{-1}}{\partial x} \frac{\partial^2 w}{\partial y \partial z}) \\ & + \text{tr}(\frac{\partial^2 w}{\partial x \partial z} \frac{\partial w^{-1}}{\partial y}) + \text{tr}(\frac{\partial^2 w}{\partial x \partial y} \frac{\partial w^{-1}}{\partial z})] dx dy dz \end{aligned}$$

Apply the compatibility condition  $\tau^* w = -w^{-1}$  in the last integral, then

$$\int_X \text{tr}(\frac{\partial^2 w}{\partial x \partial y} \frac{\partial w^{-1}}{\partial z}) dx dy dz = \int_X \text{tr}(\frac{\partial^2 w^{-1}}{\partial x \partial y} \frac{\partial w}{\partial z}) dx dy dz$$

Plug in back to the above,

$$\begin{aligned} - \int_X d \ln \det w &= \int_X \text{tr}(w^{-1}dw)^3 + 3 \int_X [\text{tr}(w^{-1} \frac{\partial^3 w}{\partial x \partial y \partial z}) + \text{tr}(\frac{\partial w^{-1}}{\partial x} \frac{\partial^2 w}{\partial y \partial z}) \\ &\quad + \text{tr}(\frac{\partial^2 w}{\partial x \partial z} \frac{\partial w^{-1}}{\partial y}) + \text{tr}(\frac{\partial^2 w^{-1}}{\partial x \partial y} \frac{\partial w}{\partial z})] dx dy dz \\ &= \int_X \text{tr}(w^{-1}dw)^3 + 3 \int_X \frac{\partial}{\partial x} [\text{tr}(w^{-1} \frac{\partial^2 w}{\partial y \partial z}) + \text{tr}(\frac{\partial w^{-1}}{\partial y} \frac{\partial w}{\partial z})] dx dy dz \\ &= \int_X \text{tr}(w^{-1}dw)^3 + 3 \int_X \frac{\partial^2}{\partial x \partial y} \text{tr}(w^{-1} \frac{\partial w}{\partial z}) dx dy dz \\ &= \int_X \text{tr}(w^{-1}dw)^3 + 3 \int_X d \text{tr} \ln w \end{aligned}$$

Use  $\ln \det w = \text{tr} \ln w$  again, we obtain

$$-4 \int_X d \ln \det w = \int_X \text{tr}(w^{-1}dw)^3$$

Finally, we restore  $\pi^2$ , which is always omitted in physics, to make the right hand side an integer,

$$- \int_X d \ln \det w = \frac{1}{4\pi^2} \int_X \text{tr}(w^{-1}dw)^3$$

□

Let us look into the formula (28), and explain why the WZW term and the Kane–Mele invariant are equivalent. On the left hand side, the determinant function is actually a section of the determinant line bundle, and it is not a global section. So the integral of the variation of  $\ln \det w$  turns out to be the jumps at the fixed points since they are isolated singularities. In other words, the result of the left integral is the alternating difference between the evaluations on the fixed points,

$$\int_X d \ln \det w = \Delta_{x_i \in X^\tau} \ln \det[w(x_i)] = \Delta_{x_i \in X^\tau} 2 \ln pf[w(x_i)]$$

where the determinant function is changed by the Pfaffian function since  $w$  is skew-symmetric at the fixed points. Since the right hand side of (28) is  $\mathbb{Z}_2$ -valued, the alternating difference can be replaced by a summation,

$$\int_X d \ln \det w = \sum_{x_i \in X^\tau} 2 \ln pf[w(x_i)]$$

On the right hand side, the topological index  $ind(w)$  or the WZW term, denoted by  $v$ , computes the topological  $\mathbb{Z}_2$  invariant.  $v$  takes the value 0 or 1, so it is an element in the additive group  $\mathbb{Z}_2$ , i.e.,  $v \in (\mathbb{Z}_2, +)$ .

The equality (28) gives rise to the congruence relation,

$$\sum_{x_i \in X^\tau} \ln pf[w(x_i)] \equiv \frac{1}{2} ind(w) \pmod{2} \quad (29)$$

If we exponentiate both sides, we obtain

$$\prod_{x_i \in X^\tau} pf[w(x_i)] = \exp\left\{ \sum_{x_i \in X^\tau} \ln pf[w(x_i)] \right\} = \exp\left\{ 2\pi i \frac{ind(w)}{2} \right\} = (-1)^{ind(w)} \quad (30)$$

where we put in a  $2\pi i$  by hand on the right hand side since it is the result of an effective field theory. In other words, the product of Pfaffians over the fixed points gives an exponentiated version of the topological  $\mathbb{Z}_2$  invariant, denoted by  $\nu$ ,

$$\nu = \prod_{x_i \in X^\tau} pf[w(x_i)] = (-1)^v \quad (31)$$

As a consequence, the exponentiated topological  $\mathbb{Z}_2$  invariant is an element in the multiplicative group  $\mathbb{Z}_2$ , i.e.,  $\nu \in (\mathbb{Z}_2, \times)$ .

By properties of the transition function  $w$ , the Pfaffian function  $pf[w(x_i)]$  only takes the value 1 or  $-1$  at any fixed point  $x_i \in X^\tau$ . So  $\nu$  does not change if we replace the Pfaffians by their signs, i.e.,

$$\nu = \prod_{x_i \in X^\tau} \text{sgn}(pf[w(x_i)])$$

As a generalization, the square root of the determinant function is added as a reference term to determine the sign of a Pfaffian, and the Kane–Mele invariant was originally defined as

$$\nu = \prod_{x_i \in X^\tau} \frac{pf[w(x_i)]}{\sqrt{\det[w(x_i)]}}$$

**Proposition 2.** *The topological  $\mathbb{Z}_2$  invariant  $\nu$  for 3d topological insulators can be computed by the topological index, i.e.,  $\text{ind}(w)$ . The Kane–Mele invariant  $\nu$  is the exponentiated topological  $\mathbb{Z}_2$  invariant, i.e.,  $\nu = (-1)^\nu$ . They are equivalent since the additive group  $(\mathbb{Z}_2, +)$  is isomorphic to the multiplicative group  $(\mathbb{Z}_2, \times)$  by the exponential map.*

The Chern–Simons invariant and the Kane–Mele invariant provide two different ways to compute the topological  $\mathbb{Z}_2$  invariant in 3d, the former is an action functional of gauge transformations and the latter is based on an effective quantum field theory. The equivalence of the Chern–Simons invariant and the Kane–Mele invariant was proved in [13, 30] from different perspectives.

## 5 Bulk-boundary correspondence

In this section, we will focus on the bulk-boundary correspondence of a time reversal invariant topological insulator, which is an index map from a different point of view. The bulk is the momentum space  $X$  and the boundary will be identified as the fixed points of the time reversal symmetry. So at the level of K-theory, the bulk theory is modeled by the  $KQ$  (or  $KR$ ) theory of  $X$ , and the boundary theory is the  $KSp$  (or  $KO$ ) theory of  $X^\tau$ . Therefore the bulk-boundary correspondence is a map connecting  $KR$ -groups, which will be realized by an index map involving a  $KKO$ -cycle.

### 5.1 Boundary theory

The phase portrait of a topological insulator is essentially determined by its behavior on the boundary. Let us look at the analytical index of the topological  $\mathbb{Z}_2$  invariant again, and identify the fixed points of the time reversal symmetry as the boundary in the geometric picture. Furthermore, the effective boundary will be the fixed point with “top codimension” by the topological index.

In the Hilbert bundle  $\pi : \mathcal{H} \rightarrow X$ , the fixed points divide the momentum space  $X$  into different coordinate patches, the chiral states  $\psi$  and  $\Theta\psi$  in a Majorana state could intersect with each other and change the chirality only at some fixed point. For a Majorana zero mode  $(\phi_0, \Theta\phi_0)$  around a fixed point  $x \in X^\tau$ , the sign of the eigenvalue of  $\phi_0$  or  $\Theta\phi_0$  can only change when passing through the fixed point  $x$ , and the spectral flow of a chiral zero mode,

i.e.,  $\psi_0$  or  $\Theta\psi_0$ , counts the existence of that Majorana zero mode. Finally, the topological  $\mathbb{Z}_2$  invariant is the parity of Majorana zero modes, which can be computed by the mod 2 spectral flow of the time reversal invariant Hamiltonian  $H$ .

At each fixed point  $x_i \in X^\tau$ , the spectral flow of a chiral zero mode around  $x_i$  gives rise to a local analytical index, which takes the value in  $KO^{-2}(x_i) = \mathbb{Z}_2$ . In total, the topological  $\mathbb{Z}_2$  invariant belongs to the summation,

$$\oplus_{x_i \in X^\tau} KO^{-2}(x_i) = KO^{-2}(X^\tau) \xrightarrow{\Sigma} KO^{-2}(pt) \ni v \quad (32)$$

where the sum  $\Sigma$  takes the collective effect (i.e., sums up then mod 2) at the end. This summation map is just the push-forward of the projection  $p : X^\tau \rightarrow pt$ . This is the discrete form of integration, then counts the parity. As a result, we identify the fixed points  $X^\tau$  as the boundary, through which information from the bulk can be exchanged. If the boundary is  $X^\tau$ , it would indeed give rise to a family index theorem, so it is better to project further to one fixed point.

Even though  $v$  is a cumulative effect over the fixed points, realizing the abstract point as a point  $x_0$ , the topological index map allows us to take only one specific fixed point  $x_0$  so that  $v \in KO^{-2}(x_0)$ . In the decomposition of  $\mathbb{S}^{1,d}$  in §2.2 or the decomposition of  $\mathbb{T}^d$  in the next example, this specific fixed point can be taken as the fixed point corresponding to the first summand, that is the point of “top codimension”. This fixed point  $x_0 \in X^\tau$  with “top codimension” is naturally identified with  $\mathbb{S}^d$  ( $d = \dim X$ ) by the Poincaré duality of K-theory.

For a  $d$ -dimensional momentum space  $X$ , the topological index map is indeed a map from KQ-theory of  $X$  to KR-theory of  $\mathbb{S}^d$ ,

$$ind_t : \widetilde{KQ}^{-i}(X) \mapsto KO^{-2}(x_0) \cong \widetilde{KR}^{-d-2}(\mathbb{S}^d) \quad (33)$$

where the isomorphism is given by the Poincaré duality in KR-theory.

**Example 22.** The  $KR$ -theory of  $\mathbb{T}^d$  can be computed based on the decomposition of the fixed points

$$(\mathbb{T}^d)^\tau = \oplus_{n=0}^d \binom{d}{n} \{pt\}$$

where  $\binom{d}{n}$  is the binomial coefficient, so that

$$KR^{-j}(\mathbb{T}^d) = \oplus_{n=0}^d \binom{d}{n} KO^{-j+n}(pt)$$

By the Poincaré duality, the spheres  $\mathbb{S}^n$  correspond to the fixed points with different codimensions so that the torus has the stable homotopy splitting

$$(\mathbb{T}^d)^\tau \sim_s \bigvee_{n=0}^d \binom{d}{n} \mathbb{S}^n$$

which is equivalent to the above decomposition. From the previous sections, we know that the topological  $\mathbb{Z}_2$  invariant only depends on the fixed point  $x_0$  with “top codimension”, i.e.,

$$v \in KO^{-j+d}(x_0) = \widetilde{KR}^{-j}(\mathbb{S}^d) \quad (34)$$

In sum, the boundary theory of a topological insulator can be modeled by  $KO^{-2}(x_0) = \widetilde{KR}^{-2-d}(\mathbb{S}^d)$ , where  $x_0$  is the fixed point with top codimension. In particular, when  $X = \mathbb{T}^2$ ,

$$v \in KO^{-2}(x_0) = \widetilde{KR}^{-4}(\mathbb{S}^2) = \widetilde{KQ}(\mathbb{S}^2)$$

Similarly, when  $X = \mathbb{T}^3$ ,

$$v \in KO^{-2}(x_0) = \widetilde{KR}^{-5}(\mathbb{S}^3) = \widetilde{KQ}^{-1}(\mathbb{S}^3)$$

## 5.2 Bulk-boundary correspondence

Once the boundary is identified as the fixed point with “top codimension”, we can talk about the bulk-boundary correspondence of a topological insulator, which is an instance of the holographic principle in condensed matter physics. The bulk-boundary correspondence at the level K-theory is supposed to be an isomorphism between the bulk K-theory and the boundary K-theory.

Let  $X$  be the momentum space of a topological insulator and  $x_0 \in X^\tau$  be the fixed point with top codimension. The bulk theory is described by the  $KQ$ -theory of  $X$ , the boundary theory is modeled by  $KO^{-2}(x_0)$  from the previous subsection. In this subsection,  $X$  is the torus  $\mathbb{T}^d$  since we want to apply the Baum–Connes isomorphism.

The Baum–Connes isomorphism or the dual Dirac isomorphism

$$KO_i(\mathbb{T}^d) = KO_i^{\mathbb{Z}^d}(\mathbb{R}^d) \simeq KO_i(C^*(\mathbb{Z}^d, \mathbb{R})) = KR^{-i}(\mathbb{T}^d, \tau) = KO_i(C(\mathbb{T}^d, \tau))$$

can be realized by an invertible real KK-class  $\beta$  in  $KKO(C_{\mathbb{R}}(\mathbb{T}^d), C(\mathbb{T}^d, \tau))$  connecting the real K-homology groups of  $C_{\mathbb{R}}(\mathbb{T}^d)$  and  $C(\mathbb{T}^d, \tau)$ , i.e.,

$$KO_i(\mathbb{T}^d) \times KKO(C_{\mathbb{R}}(\mathbb{T}^d), C(\mathbb{T}^d, \tau)) \xrightarrow{\sim} KO_i(C(\mathbb{T}^d, \tau))$$

Let  $\alpha$  be the inverse of  $\beta$ , that is,  $\alpha \in KKO(C(\mathbb{T}^d, \tau), C_{\mathbb{R}}(\mathbb{T}^d))$  such that  $\alpha \circ \beta = id$ , so  $\alpha$  realizes the Dirac isomorphism

$$KR^{-i}(\mathbb{T}^d, \tau) \times KKO(C(\mathbb{T}^d, \tau), C_{\mathbb{R}}(\mathbb{T}^d)) \xrightarrow{\cong} KO_i(\mathbb{T}^d)$$

If  $i_0 : x_0 \hookrightarrow \mathbb{T}^d$  is the inclusion map, then it induces the restriction map in  $KO$ -theory

$$i_0^* : KO^{-j}(\mathbb{T}^d) \rightarrow KO^{-j}(x_0)$$

**Proposition 3.** *The bulk-boundary correspondence of a topological insulator is a special case of the following composition map, denoted by  $\eta$ ,*

$$\eta := i_0^* \circ PD \circ \alpha : \widetilde{KR}^{-i}(\mathbb{T}^d) \cong \widetilde{KO}_i(\mathbb{T}^d) \cong \widetilde{KO}^{d-i}(\mathbb{T}^d) \rightarrow KO^{d-i}(x_0) \quad (35)$$

where the middle isomorphism is the Poincaré duality. More precisely, when  $d = 2$  and  $i = 4$ , the bulk-boundary correspondence of a 2d topological insulator is the isomorphism

$$\eta : \widetilde{KQ}(\mathbb{T}^2) = \widetilde{KR}^{-4}(\mathbb{T}^2) \xrightarrow{\cong} KO^{-2}(x_0)$$

Similarly, when  $d = 3$  and  $i = 5$ , the bulk-boundary correspondence of a 3d topological insulator is the isomorphism

$$\eta : \widetilde{KQ}^{-1}(\mathbb{T}^3) = \widetilde{KR}^{-5}(\mathbb{T}^3) \xrightarrow{\cong} KO^{-2}(x_0)$$

If we identify  $KO^{d-j}(x_0)$  with  $KR^{-j}(\mathbb{S}^d)$  by the Poincaré duality, then the bulk-boundary correspondence will be rephrased as

$$\eta = i^* : \widetilde{KR}^{-j}(\mathbb{T}^d) \rightarrow \widetilde{KR}^{-j}(\mathbb{S}^d)$$

where  $i : \mathbb{S}^d \hookrightarrow \mathbb{T}^d$  is the inclusion map based on the stable homotopy splitting of  $\mathbb{T}^d$ .

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